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METHODS

The present invention relates to protein kinase catalytic domain structures and mutants and screening assays making use thereof.

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) is a key protein kinase, regulating activity of a group of related protein kinases through phosphorylation. These kinases include isoforms of Protein Kinase B (also known as Akt) [Brazil and Hemmings, 2001, Scheid and Woodgett, 2001], p70 ribosomal S6 kinase (S6K) [Alessi et al., 1997, Volarevic and Thomas, 2001], p90 ribosomal S6 Kinase (RSK) [Frodin and Gammeltoft, 1999] and the serum and glucocorticoid induced-protein kinase (SGK) [Lang and Cohen, 2001]. These enzymes are stimulated by hormones and growth factors and phosphorylate regulatory proteins mediating the various physiological effects of these agonists.

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PDK1 possesses an N-terminal kinase catalytic domain and a C-terminal pleckstrin homology (PH) domain [Alessi et al., 1997, Stephens et al., 1998]. PDK1 activates its substrates by phosphorylating these kinases at their activation loop (reviewed in [Alessi, 2001, Toker and Newton, 2000]). The phosphorylation of PKB by PDK1 is dependent upon prior activation of the phosphoinositide 3-kinase (PI-3-kinase) and the production of the second messenger, phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P₃) which binds to the PH domains of PDK1 and PKB. This does not activate either PKB or PDK1 but instead recruits and co-localises these enzymes at the plasma membrane.

25 plasma membrane.

Unlike PKB, the other PDK1 substrates described thus far do not interact with PtdIns(3,4,5)P₃ nor is the rate at which they are phosphorylated by PDK1 further enhanced by the binding of PDK1 to PtdIns(3,4,5)P₃. Instead the ability of PDK1 to phosphorylate S6K, SGK and RSK is promoted by

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phosphorylation of these enzymes at a residue located C-terminal to the kinase catalytic domain in a region known as the hydrophobic motif [Alessi et al., 1997, Kobayashi and Cohen, 1999, Pullen et al., 1998]. The kinases that phosphorylate the hydrophobic motif of S6K and SGK are unknown but as the phosphorylation of this residue *in vivo* is dependent on PI-3-kinase activation, the hydrophobic motif kinases and/or the hydrophobic motif phosphatases may be regulated by PtdIns(3,4,5)P₃. In the case of RSK isoforms, phosphorylation by the ERK1/ERK2 MAP kinases induce phosphorylation of the hydrophobic motif (reviewed in Frodin and Gammeltoft, 1999).

PDK1 belongs to the same subfamily of protein kinases as its substrates, termed the AGC protein kinases as they are related to the cAMP dependent protein kinase (PKA)/cGMP dependent protein kinase/Protein kinase C (PKC). PKA is the only AGC kinase whose crystal structure has been solved. Like all protein kinases, its catalytic core possesses an N-terminal lobe consisting mainly of β -sheet and a predominantly α -helical Cterminal lobe [Taylor et al., 1992, Husen and Kuriyan, 2002]. The ATP binding site is located in between the 2 lobes [Johnson et al., 2001, Knighton et al., 1991]. At the very C-terminus, PKA possesses an extended loop that terminates in the sequence FXXF which resembles the first part of the hydrophobic motif phosphorylation site of S6K and SGK (FXXFS/TY) in which the Ser/Thr is the phosphorylated residue [Biondi et al., 2000]. In the structure of PKA, the FXXF motif is buried in a hydrophobic pocket in the small lobe of the PKA catalytic domain [Knighton et al., 1991] and mutation of either of the Phe residues drastically reduces PKA activity towards a peptide substrate [Etchebehere et al., 1997]. Unlike other AGC kinases, PDK1 does not possess a hydrophobic motif C-terminal to its catalytic domain. However, there is evidence that PDK1 possesses a hydrophobic pocket in the small lobe of its catalytic domain similar to that

in PKA. We have biochemically demonstrated that the interaction of PDK1 with four of its substrates (S6K1, SGK1, PKζ and PKC related kinase-2 (PRK2)) is reduced or abolished by mutation of residues predicted to form part of this pocket [Balendran et al., 2000, Biondi et al., 2000]. Furthermore, mutation of a central residue in the predicted pocket, Leu 155, prevented PDK1 from phosphorylating and activating S6K1 and SGK1 without affecting its ability to phosphorylate either PKB or a short peptide substrate that encompasses the activation loop of PKB (T308tide) [Biondi et al., 2000]. The hydrophobic pocket on the kinase domain of PDK1 has been termed the "PIF-pocket" after the name of the first AGC-kinase hydrophobic motif-containing peptide (PDK1 Interacting Fragment) that was found to bind PDK1 [Balendran et al., 1999a]. It has been suggested that the PIF-pocket in PDK1 functions as a docking site, enabling PDK1 to interact with some of its.physiological substrates. Furthermore, there is evidence that phosphorylation of the hydrophobic motif of S6K1, SGK and RSK2 [Balendran et al., 1999b, Biondi et al., 2001, Frodin et al., 2000] promotes the interaction of these enzymes with PDK1. These findings suggest that the PIF-pocket on PDK1 could contain a phosphate binding site promoting the binding of PDK1 to a subset of substrates (S6K, SGK and RSK) once these enzymes have been phosphorylated at their hydrophobic motif. This would result in a physiological phosphate dependent interaction. In addition there is evidence that occupancy of the PIF-pocket activates PDK1 as peptides that encompass the hydrophobic motif of PRK2 [Biondi et al., 2000] and RSK [Frodin et al., 2000] induce a 4-6-fold activation of PDK1.

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Previous predicted structures PDK1 catalytic domain were obtained using homology modelling methods based upon structural information available from the catalytic domain of PKA (Biondi et al., 2000). These predictions of the PDK1 catalytic domain structure were thus biased towards the catalytic domain from which the structural information was obtained.

We have determined a crystal structure for the kinase domain of the AGC family protein kinase PDK. The structure defines the PIF-pocket and reveals an adjacent possible phosphate binding site. Furthermore, we have performed structure-based mutagenesis and biochemical analysis which support the existence of such a phosphate-binding site. This may mediate the phosphate dependent docking interaction with substrates such as (for PDK1) S6K and SGK. We have used a novel algorithm to define the conformational state of the crystallised PDK1 relative to all the reported structures of PKA, which shows that while PDK1 has all the signs of being in an active form in the crystal, its overall conformation is in-between and 'open' and 'closed' state. We have also determined crystal structures for the kinase domain of PDK1 in complex with modulators of PDK1 activity. On the basis of this work we provide drug screening methods and mutated protein kinase molecules (which are useful in, for example, drug screening methods).

A first aspect of the invention provides a method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

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The term PDK1 as used herein includes a polypeptide (a PDK1 polypeptide) comprising the amino acid sequence identified as PDK1 in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776-789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714, or a variant, fragment, fusion or derivative thereof, or a fusion of a said variant or fragment or derivative, for example as described in WO98/41638, incorporated herein by reference. It is preferred that the said PDK1 polypeptide is a protein kinase. It is preferred that the said PDK1 polypeptide is a protein kinase that is capable of phosphorylating a threonine residue that lies in a Thr-Phe-Cys-Gly-Thr-Xaa-Glu-Leu consensus motif (where the underlined Thr corresponds to the threonine that is phosphorylated by PDK1 and Xaa is a variable residue), and preferably that is capable of phosphorylating PKB, for example PKBa, at residue Thr308. The rate at which the said PDK1 polypeptide is capable of phosphorylating a threonine residue as described above may be increased in the presence of PtdIns(3,4,5)P3 or PtdIns(3,4)P2 but it will be appreciated The said polypeptide may be capable of that this is not essential. phosphorylating the equivalent residues to Thr308 of PKBa on PKC isoforms (LeGood et al (1998) Science 281: 2042-2045; et al (1998) Curr. Biol. 8: 1069-1077; Dutil et al (1998) Curr. Biol. 8:1366-1375), p70 S6 kinase (Alessi et al (1998) Curr. Biol. 8: 69-81; Pullen et al (1998) Science 279, 707-710), SGK (sequence given in Webster et al (1993) Mol. Cell. Biol. 13, 1031-2040; equivalent residues identified in US application no 112217 filed on 14 December 1998; GB 9919676.8, filed on 19 August 1999, and Kobayashi & Cohen (1999)) and PKA (Cheng et al (1998) Proc. Natl. Acad. Sci. USA 95: 9849-9854). It may further be preferred that the substrate specificity and/or other characteristics of the said PDK1 polypeptide in vitro may be substantially as reported in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 77610

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789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714.

We have found that a fragment of PDK1 consisting essentially of residues equivalent to residues 51 to 359 of full length human PDK1 is particularly beneficial for determining a structure for the catalytic domain of PDK1. This fragment has, for example, protein kinase activity and surprisingly beneficial solubility and stability characteristics which make it particularly suitable for structural studies, for example formation of crystals which may be analysed by X-ray crystallography methods. Other fragments of PDK1 were surprisingly found to be unsuitable for crystallisation, as discussed in Example 5.

It is particularly preferred that the structure is one determined for the fragment consisting of residues 51 to 359 of full length human PDK1. The fragment may comprise an N-terminal or C-terminal fusion polypeptide (ie amino acid sequence not derived from PDK1), though this is preferably of less than or equal to about 10, 5, 4, 3, 2 or 1 amino acids. For example, it is particularly preferred that the structure is one determined for a polypeptide consisting residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro (or less preferably other sequence forming part of a protease cleavage site) preceding the methionine corresponding to Met51 of human PDK1. A further preferred structure is one determined for the fragment consisting essentially of residues 71 to 359 of full length human PDK1 (or residues equivalent thereto), which also has protein kinase activity.

It is particularly preferred that the structure is one determinable by a method as described in Example 1, for example a structure obtainable by X-ray analysis from a crystal obtainable using a mother liquor solution comprising

ammonium sulphate, preferably between 1.8 and 2.2M. It is particularly preferred that the mother liquor solution is of pH 7 to 9, preferably 7 to 8.5, most preferably pH8.5, and comprises ammonium sulphate and preferably ATP. Crystals may form in the absence of ATP but better crystals may be obtained in the presence of ATP. Preferably the crystal is obtainable using a mother liquor solution containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP. Further preferred details of the crystallisation and X-ray analysis are described in Example 1, for example as partially summarised in Table 1 (shown in Example 1).

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It is particularly preferred that the structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure based or modelled on such a structure or co-ordinates. The co-ordinates shown in Example 2 are for the PDK1 fragment with all alternate side chains. The co-ordinates shown in Example 3 are for the PDK1 fragment without alternate side chains. The co-ordinates shown in Example 4 are for the dimer of the PDK1 fragment, without alternate side chains; chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

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The structure may be one determined following crystallisation in the presence of a known or potential interactor with PDK1 or modulator of PDK1 activity (as discussed further below), for example a known or potential inhibitor of PDK1 activity. For example, the structure may be one determined following crystallisation in the presence of a known protein kinase inhibitor, for example an inhibitor that binds at the ATP binding site, for example an ATP-competitive inhibitor, for example staurosporine or a staurosporine derivative, for example UCN-01. Examples of such crystallisation techniques and analysis are given in Example 6, and examples of co-ordinates are given in Examples 7 and 8. It will be

appreciated that some variation in crystallisation conditions (for example different mother liquors) may be required for co-crystallisation with different molecules. Techniques for investigating suitable crystallisation conditions in each case will be well known to those skilled in the art.

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A further aspect of the invention provides a crystalline form of a polypeptide as defined in any of the preceding aspects of the invention, for example a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof; a polypeptide consisting of residues 51 to 359 of full length human PDK1 or a fusion thereof; a polypeptide consisting of residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro preceding the methionine corresponding to Met51 of human PDK1; a polypeptide consisting of residues 71 to 359 of full length human PDK1 or a fusion thereof.

The crystalline form may further comprise co-crystallised molecule, for example a known or potential interactor with PDK1 or modulator of PDK1 activity, or a test compound whose properties vis a vis PDK1 may not be known. For example, the co-crystallised molecule, for example test compound, may be a molecule that is known to modulate protein kinase activity, or may already be known to modulate PDK1 protein kinase activity. For example, the co-crystallised molecule may be staurosporine, the staurosporine derivative UCN-01 (7-hydroxyl staurosporine) or other

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staurosporine derivative.

Such co-crystallisation and structures determined from co-crystallised molecules may be useful in molecular modelling and in determining features of the polypeptide and compound that are important for interaction.

This may be useful in designing or selecting further test compounds, for example as discussed in Example 6.

In one embodiment it is preferred that the modelled molecule is predicted to bind to a region of the structure termed the "PIF binding pocket", the "phosphate binding pocket" and/or the α C helix (residues equivalent to 123-136 of full length human PDK1), particularly the residue equivalent to Arg 131 of full length human PDK1, or interacting regions. As discussed in Example 1, the PIF binding pocket is considered to be formed by residues including Lys115, Ile118, Ile119 on the αB helix, Val124, Val127 on the αC helix and Leu 155 on β-sheet 5. The phosphate binding pocket is considered to be formed by residues including Lys76, Arg 131, Thr 148 and Gln150. Residues of the αC helix that are considered to interact either with phosphate bound in the phosphate binding site or intermolecularly with phosphorylated Ser241 of PDK1 include Arg131 (phosphate binding site) and Arg 129 and His126 (phosphorylated Ser241). Glu 130 is involved in binding the α-phosphate of the bound ATP, and Val124 and Val127 form part of the PIF binding pocket, as discussed in Example 1.

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It is preferred that the compound is for modulating the protein kinase activity of PDK1. The protein kinase activity of PDK1 that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu ("PDK1" activity). Alternatively or in addition, the modulated activity may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Phe-Xaa-Xaa-Phe-Ser/Thr-Phe/Tyr ("PDK2" activity). The substrate polypeptide may be, for example, a PKB, SGK, p70 S6 kinase, PKC or (in relation only to phosphorylation of the underlined residue in a polypeptide with the amino acid sequence <a href="Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Phe-Cys-Gly-Thr-X

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Glu-Leu) PKA polypeptide. The modulated protein kinase activity may be towards PKB or other PH-domain-comprising/phosphoinositide-binding substrate of PDK1; or SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif" FXXFS/TY; or an artificial substrate such as T308tide (which comprises the sequence of PKB which is phosphorylated by PDK1) or PDKtide (which comprises the sequence of PKB which is phosphorylated by PDK1 (eg T308tide) fused to a sequence mimicking a phosphorylated hydrophobic motif ie FXXFZY, in which Z is a negatively charged (for example acidic) residue (eg PIFtide)). Such substrates for PDK1 are discussed, for example, in WO 01/44497. Other activities of PDK1 that may be modulated include interactions with other polypeptides or phosphoinositides and/or intramolecular interactions.

It is preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of the PDK1 is a three-dimensional structure of at least a part of the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, and a compound that is predicted to interact with the said PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1 is selected. Alternatively, the compound may bind to a portion of said PDK1 polypeptide that is not the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, for example so as to interfere with the binding of the ATP or substrate polypeptide or their access to the catalytic site. In a still further example, the compound may bind to a portion of PDK1 so as to decrease said polypeptide's activity by an allosteric effect. This allosteric effect may be an allosteric effect that is involved in the natural regulation of PDK1's activity.

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It is further preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure of the part of the protein kinase catalytic domain of PDK1 that is defined by residues Lys115, Ile118, Ile119 (on the αB helix), Val124, Val127 (on the αC helix) and Leu 155 (on β -sheet 50 and/or residues Lys76, Arg 131, Thr 148 and Gln150 and/or residues Arg131, Arg 129, His126, Glu 130 of full-length human PDK1 and a compound that is predicted to interact with the said part of the protein kinase catalytic domain is selected.

For example, it is preferred if the portions of the structure of PDK1 shown in Figures 1 and 2 as forming the PIF binding pocket and/or phosphate binding pocket and/or αC helix interactions (for example with phosphoserine241) are compared with the structure of the candidate compound.

A further aspect of the invention provides a method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1. that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of a compound is compared with a

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three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, is selected.

The three-dimensional structure of a compound may be compared with the three-dimensional structure of the hydrophobic and/or phosphate binding pocket and/or αC helix or region interacting therewith, as appropriate. A compound that can interact with the hydrophobic pocket and/or phosphate binding pocket, in particular residues noted above as defining such regions, in a similar manner (for example similar separation and/or type of interaction ie hydrophobic or ionic, and/or similar cumulative energy of interaction) to an interacting polypeptide such as S6K-pHM may be selected. Methods of assessing the interaction are well known to those skilled in the art and are discussed further below.

The three-dimensional structures that are compared may be, as appropriate, predicted or modelled three-dimensional structures (for example on the basis of a PDK1 structure as referred to above, for example as represented by the co-ordinates given in Examples 2, 3 or 4 or 6 or 7) or may be three-dimensional structures that have been determined, for example by techniques such as X-ray crystallography, as well known to those skilled in the art. The three-dimensional structures may be displayed by a computer in a two-dimensional form, for example on a computer screen. The comparison may be performed using such two-dimensional displays.

The following relate to molecular modelling techniques: Blundell et al (1996) Stucture-based drug design Nature 384, 23-26; Bohm (1996)

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Computational tools for structure-based ligand design Prog Biophys Mol Biol 66(3), 197-210; Cohen et al (1990) J Med Chem 33, 883-894; Navia et al (1992) Curr Opin Struct Biol 2, 202-210.

The following computer programs, for example, may be useful in carrying 5 out the method of this aspect of the invention: GRID (Goodford (1985) JMed Chem 28, 849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al (1991) Proteins: Structure, Function and Genetics 11, 29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al (1990) Proteins: Structure, Function and 10 Genetics 8, 195-202; available from Scripps Research Institute, La Jolla, CA); DOCK (Kuntz et al (1982) J Mol Biol 161, 269-288; available from the University of California, San Francisco, CA); LUDI (Bohm (1992) J Comp Aid Molec Design 6, 61-78; available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al (1991) Tetrahedron 47, 8985; 15 available from Molecular Simulations, Burlington, MA); LeapFrog (available from Tripos Associates, St Louis, MO); Gaussian 92, for example revision C (MJ Frisch, Gaussian, Inc., Pittsburgh, PA ©1992); AMBER, version 4.0 (PA Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, 20 MA ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, CA ©1994). Programs may be run on, for example, a Silicon Graphics™ workstation, Indigo²™ or IBM RISC/6000™ workstation model 550.

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Several in silico methods could be employed, for example, via a substructure search for new ligands using programmes such as CHEM DRAW or CHEM FINDER. The basic structure of the natural ligand (for example a phosphorylated hydrophobic motif peptide such as S6K-pHM) capable of binding to PDK1 (or other protein kinase) is taken (or predicted)

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and various structural features of it (for example the hydrophobic and negatively charged entities) are submitted to a programme which will searches a set of chemical company catalogues for chemicals containing this substructure.

- These compounds are then screened by eye for groups that could not 5 PIF/phosphate binding pockets interact with the (or residues/interacting region) because, for example, they are too large or have steric or charge hindrance, and those are discarded. The remaining chemicals are submitted to a PRODRG server and topologies/co-ordinates for these chemicals are created. These chemicals are modelled into the 10 structure, from which chemicals that are possibly able to bind to the PIF/phosphate binding site domain/αC helix/interacting region are selected. details of the PRODRG programme are available http://davapc1.bioch.dundee.ac.uk/programs/prodrg/prodrg.html.
- These compounds may then be ordered or synthesised and assessed, for one or more of ability to bind to and/or modulate PDK1 (or other protein kinase) activity. The compounds may be crystallised with the PDK1 or other protein kinase protein and the structure of any complex determined, as illustrated in Examples 6 to 8.
- An alternative approach is to use PRODRG: a tool for generating GROMOS/MOL2/WHATIF topologies and hydrogen atom positions from small molecule PDB files. We take the natural ligand and computationally vary all possible groups at each site on the ligand, with a variety of new groups while the protein co-ordinates and the ligand back-bone co-ordinates remain fixed the results can then be screened for hindrance and repulsion, and the molecules are obtained either through catalogues or made.

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As noted above, the selected or designed compound may be synthesised (if not already synthesised) or purified and tested for its effect on the relevant hydrophobic/phosphate pocket-containing protein kinase, for example its effect on the protein kinase activity. The compound may be tested in a screening method of the invention or other screening method. The compound may be formulated for pharmaceutical use, for example for use in *in vivo* trials in animals or humans, or for use in agriculture, for example as an antifungal agent.

It may be useful to analyse a protein kinase structure (for example a structure determined or predicted for a complex of the protein kinase with a binding partner) in order to determine the activation state of the structure. This may be useful in further modelling binding of the binding partner to the protein kinase in other activation states, and in predicting how the binding partner may affect the activation state of the protein kinase or compete with other potential binding partners. It may also be useful in designing and assessing derivatives of the binding partner.

Thus, a further aspect of the invention provides a method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates. The method may further comprise the step of classifying the activation state of the structure as "open", "closed" or "intermediate". Details of the analysis, which involves the generation of eigenvectors and associated eigenvalues are given in Example 1. The analysis makes use of techniques described in Amadei et al (1993) Essential dynamics of proteins. Proteins 17, 412-425.

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The hydrophobic/phosphate pocket-containing protein kinase may be PDK1. Alternatively, it may be an isoform of Serum and Glucocorticoid

stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2. Hydrophobic/phosphate pocket-containing protein kinases and their EMBL database accession numbers are listed in Table I. Sequences considered to form the phosphate binding pocket from representative hydrophobic/phosphate pocket-containing protein kinases are shown in Figure 5. All AGC family protein kinases other than PKA may be hydrophobic/phosphate pocket-containing protein kinases, as defined above. In addition to the protein kinases shown in Figure 7, rhodopsin and G-protein coupled receptor protein kinases, for example, may possibly also have a hydrophobic/phosphate pocket as defined above.

The terms SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, for example, as used herein include a polypeptide (a SGK, PKB, PKA, p70S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 polypeptide) comprising the amino acid sequence identified as a SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, respectively, in the relevant EMBL database records indicated in Table 2.

Table 2

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Activation or T- AGC Ac	cession
Loop Hydrophobic nu	mber
Motif	
consensus: <u>TFCGTxxYxAPD</u> FxxF <u>S</u> Y	
L E Y <u>T</u> F	
PKB α <u>T</u> FCGTPEYLAPE FPQF <u>S</u> Y (Y150	56)
PKBβ <u>T</u> FCGTPEYLAPE FPQF <u>S</u> Y (P3175	51)
PKBγ <u>T</u> FCGTPEYLAPE FPQF <u>S</u> Y (AF13	5794)
SGK1 <u>T</u> FCGTPEYLAPE FLGF <u>S</u> Y (AAD	41091)

SGK2	<u>T</u> FCGTPEYLAPE	FLGF <u>S</u> Y	(AF169034)
SGK3	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	FLGF <u>S</u> Y	(AF169035)
PKCa `	<u>T</u> FCGTPDYIAPE	$\mathtt{FEGF}\underline{\mathtt{S}}\mathtt{Y}$	(4506067)
РКСВІ	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	fagf <u>s</u> y	(4506069)
РКСВП	TFCGTPDYIAPE	fegf <u>s</u> f	(P05127)
РКСу	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	$\mathtt{FGGF}\underline{\mathtt{T}}\mathtt{Y}$	(P05129)
РКСδ	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	fagf <u>s</u> f	(5453970)
РСКС	TFCGTPNYIAPE	FEGFEY	(4506079)
PKCı	<u>T</u> FCGTPNYIAPE	FEGFEY	(4506071)
PRK1	TFCGTPEFLAPE	FLDFDF	(AAC50209)
PRK2	TFCGTPEFLAPE	FRDFDY	(AAC50208)
p70-S6Kα	TFCGTIEYMAPE	$\mathtt{FLGF}\underline{\mathtt{T}}\mathtt{Y}$	(AAA36410)
p70-S6Kβ	TFCGTIEYMAPE	$\mathtt{FLGF}\underline{\mathtt{T}}\mathtt{Y}$	(4506739)
p90-RSK1	<u>S</u> FCGTVEYMAPE	frgf <u>s</u> f	(138556)
p90-RSK2	<u>S</u> FCGTVEYMAPE	frdf <u>s</u> f	(P51812)
p90-RSK3	<u>S</u> FCGTIEYMAPE	frgf <u>s</u> f	(CAA59427)
MSK1	$\underline{\mathtt{S}}\mathtt{F}\mathtt{C}\mathtt{G}\mathtt{T}\mathtt{I}\mathtt{E}\mathtt{Y}\mathtt{M}\mathtt{A}\mathtt{P}\mathtt{D}$	FQGY <u>S</u> F	(AAC31171)
MSK2	<u>S</u> FCGTIEYMAPE	FQGY <u>S</u> F	(AAC67395)
PDK1	<u>S</u> FVGTAQYVSPE	(1)	(AF017995)

Table 2. Alignment of the amino acid sequences surrounding the T-loop and the hydrophobic motif of AGC kinases. All the sequences and accession numbers are from human proteins. The underlined residues correspond to those that become phosphorylated. Footnotes: (1) PDK1 does not possess a hydrophobic motif.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the

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protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor et al (1999) Curr Biol 9, 186-197.

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The PDK1 may also be a polypeptide with the amino acid sequence of residues 51 to 359 or 404 (or 71 to 360) of full-length human PDK1; this may comprise the protein kinase domain of PDK1, as described in Example 2. The PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may also be Myc epitope-tagged or His-tagged, as described in Example 1. The p70 S6 kinase, for example, may have a His tag at its N-terminus and/or may lack the carboxy terminal 104 residues (p70 S6K-T2). The PDK1 or SGK may be a Saccharomyces cerevisiae homologue, for example Pkh1 or Pkh2 (PDK1 homologues) or Ypk1 or Yrk2 (SGK homologues), as described in Casamayor et al (1999) Curr Biol 9, 186-197.

It is particularly preferred, although not essential, that the variant or fragment or derivative or fusion of the PDK1, or the fusion of the variant or fragment or derivative has at least 30% of the enzyme activity of full-length human PDK1 with respect to the phosphorylation of full-length human PKBα on residue Thr308 or SGK1 on residue Thr 256 in either the presence or absence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂. It is more preferred if the variant or fragment or derivative or fusion of the said protein kinase, or the fusion of the variant or fragment or derivative has at least 50%, preferably at least 70% and more preferably at least 90% of the enzyme activity of

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PDK1 with respect to the phosphorylation of PKBα or SGK1. However, it will be appreciated that variants or fusions or derivatives or fragments which are devoid of enzymatic activity may nevertheless be useful, for example by interacting with another polypeptide. Thus, variants or fusions or derivatives or fragments which are devoid of enzymatic activity may be useful in a binding assay, which may be used, for example, in a method of the invention in which modulation of an interaction of a mutated PDK1 of the invention and optionally also PDK1 with a interacting polypeptide or compound, for example an interacting polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr, for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Asp/Glu-Phe/Tyr or Phe/Tyr-Xaa-Xaa-Phe/Tyr-PhosphoSer/PhosphoThr-Phe/Tyr is measured.

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15 It is preferred that the variant or fragment or derivative or fusion of the said hydrophobic/phosphate binding pocket-containing protein kinase, or the fusion of the variant or fragment or derivative comprises a hydrophobic pocket and a phosphate binding pocket in the position equivalent to the hydrophobic and phosphate binding pocket of human PDK1, as discussed further below.

Equivalent preferences apply to a variant or fragment or derivative or fusion of the SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 (for example), or the fusion of the variant or fragment or derivative, with the substitution in relation to SGK, PKB and p70S6 kinase of the peptide substrate Crosstide (GRPRTSSFAEG), or for PKB and SGK of the peptide substrate RPRAATF; the substitution in relation to PKA of the peptide substrate Kemptide (LRRASLG); the substitution in relation to PKC isoforms and PRK1/2 of histone H1; and the substitution in relation to MSK1/2 or p90-RSK1/2/3 of CREBtide (EILSRRPSYRK).

By "variants" of a polypeptide we include insertions, deletions and substitutions, either conservative or non-conservative. In particular we include variants of the polypeptide where such changes do not substantially alter the activity of the said polypeptide, for example the protein kinase activity of PDK1, as described above.

By "conservative substitutions" is intended combinations such as Gly, Ala; Val, Ile, Leu; Asp, Glu; Asn, Gln; Ser, Thr; Lys, Arg; and Phe, Tyr.

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The three-letter amino acid code of the IUPAC-IUB Biochemical Nomenclature Commission is used herein, with the exception of the symbol Zaa (negatively charged amino acid). In particular, Xaa represents any amino acid. It is preferred that Xaa and Zaa represent a naturally occuring amino acid. It is preferred that at least the amino acids corresponding to the consensus sequences defined above are L-amino acids.

It is particularly preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of PDK1 referred to above (or the sequence for SGK (including SGK1, 2 and 3), PKB, PKA or p70 S6 kinase, for example, as appropriate, referred to above), more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 80%, in further preference at least 85%, in still further preference at least 90% and most preferably at least 95% or 97% identity with the amino acid sequence defined above.

It is still further preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase, as

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defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of the catalytic domain, particularly the residues forming the hydrophobic pocket, of PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) in the appropriate sequence referred to above, more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 80%, in further preference at least 83 or 85%, in still further preference at least 90% and most preferably at least 95% or 97% identity with the amino acid sequence defined above. It will be appreciated that the catalytic domain of a protein kinase-related polypeptide may be readily identified by a person skilled in the art, for example using sequence comparisons as described below.

The percent sequence identity between two polypeptides may be determined using suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group and it will be appreciated that percent identity is calculated in relation to polypeptides whose sequence has been aligned optimally.

The alignment may alternatively be carried out using the Clustal W program (Thompson *et al* (1994) *Nucl Acid Res* 22, 4673-4680). The parameters used may be as follows:

Fast pairwise alignment parameters: K-tuple(word) size; 1, window size; 5, gap penalty; 3, number of top diagonals; 5. Scoring method: x percent.

Multiple alignment parameters: gap open penalty; 10, gap extension penalty; 0.05.

Scoring matrix: BLOSUM.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as

the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor et al (1999) Curr Biol 9, 186-197.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide that is capable of interacting with a polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr, preferably Phe-Xaa-Xaa-Phe/Tyr, more preferably Phe-Xaa-Xaa-Phe, still more preferably Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr or Phe/Tyr-Xaa-Xaa-Phe/Tyr-COOH, for example the polypeptide PIF or PIFtide, as defined below. Further preferences for the said polypeptide are as given above.

The protein kinase activity of PKB, SGK or p70 S6 kinase that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Arg-Xaa-Arg-Xaa-Xaa-Ser/Thr. The polypeptide may be Glycogen Synthase Kinase 3 (GSK3), 40 S ribosomal subunit S6, BAD, 6-phosphofructo-2-kinase, phosphodiesterase3b, human caspase 9, endothelial nitric oxide synthase or BRCA1.

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A compound identified by a method of the invention may modulate the ability of the protein kinase to phosphorylate different substrates, for example different naturally occurring polypeptides, to different extents. The compound may inhibit the protein kinase activity in relation to one substrate but may increase the protein kinase activity in relation to a second substrate.

For example, the protein kinase activity of PDK1 may be modulated to a different extent for PKB when compared with SGK, p70 S6 kinase and/or PKC.

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It will be appreciated that the modulatory, for example inhibitory action of a compound found to bind (or inhibit binding of a polypeptide or compound) to the protein kinase may be confirmed by performing an assay of enzymic activity (for example PDK1 and/or PDK2 protein kinase activity) in the presence of the compound.

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By "hydrophobic pocket-containing protein kinase having a hydrophobic pocket (PIF binding pocket) in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150," is meant a polypeptide having an amino acid sequence identifiable as that of a protein kinase catalytic domain, and further having a predicted or determined three-dimensional structure that includes a hydrophobic pocket corresponding to the region indicated in Example 1 as the PIF binding pocket, and a pocket corresponding to the region indicated in Example 1 as the phosphate binding pocket. The hydrophobic pocket and phosphate binding pockets in PDK1 do not overlap with the ATP or phosphorylation site binding sites on PDK1.

It is preferred that the protein kinase has identical or conserved residues that are equivalent to Lys 115, Ile118, Ile119, Val124, Val127 and/or Leu 155 of human PDK1, more preferably at least Lys115 and Leu155 of human PDK1, most preferably an identical residue equivalent to Leu155. Thus, for

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example, the protein kinase may have a Lys residue at the position equivalent to Lys115 of PDK1 and/or a Leu residue at the position equivalent to Leu155 of PDK1. It is preferred that the protein kinase does not have an Ala at the position equivalent to Lys115 and/or a Ser, Asp or Glu at the position equivalent to Leu155 of PDK1.

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It is further preferred that the protein kinase has identical or conserved residues that are equivalent to Lys76, Arg131, Thr148 and/or Gln 150 of human PDK1, more preferably at least Lys76 and Gln150 of human PDK1, most preferably an identical residue equivalent to Gln150. Figure 5B shows an alignment of examples of protein kinases considered to have a phosphate binding pocket at the position equivalent to the said phosphate binding pocket of PDK1. Sequence conservation/preferred residues at the positions identified are discussed further in Example 1.

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An amino acid sequence may be identifiable as that of a protein kinase catalytic domain by reference to sequence identity or similarities of three dimensional structure with known protein kinase domains, as known to those skilled in the art.

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Protein kinases show a conserved catalytic core, as reviewed in Johnson et al (1996) Cell, 85, 149-158 and Taylor & Radzio-Andzelm (1994) Structure 2, 345-355. This core folds into a small N-terminal lobe largely comprising anti-parallel β -sheet, and a large C-terminal lobe which is mostly α -helical. A deep cleft at the interface between these lobes is the site of ATP binding, with the phosphate groups near the opening of the cleft.

Protein kinases also show conserved sequences within this catalytic core, and the residue equivalent to a given residue of, for example, PDK1, may be identified by alignment of the sequence of the kinase with that of known

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kinases in such a way as to maximise the match between the sequences. The alignment may be carried out by visual inspection and/or by the use of suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group, which will also allow the percent identity of the polypeptides to be calculated. The Align program (Pearson (1994) in: Methods in Molecular Biology, Computer Analysis of Sequence Data, Part II (Griffin, AM and Griffin, HG eds) pp 365-389, Humana Press, Clifton).

- The comparison of amino acid sequences or three dimension structure (for example from crystallography or computer modelling based on a known structure) may be carried out using methods well known to the skilled man, for example as described in WO 01/44497.
- MAP kinase, MEK1, Cdk2 and Erk2 (for example) are not protein kinases having a hydrophobic pocket in the position equivalent to the hydrophobic (PIF binding) pocket of PDK1. MEK1, Cdk2 and ERK2 may have a larger hydrophobic pocket which interacts with an amino acid sequence motif (which may be Phe-Xaa-Phe-Pro) which is not Phe-Xaa-Xaa-Phe. Thus, these protein kinases do not have a hydrophobic pocket in the position equivalent to the said hydrophobic (PIF-binding) pocket of PDK1.

A further aspect of the invention provides a mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues

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equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated. It is preferred that the said protein kinase is PDK1. The said protein kinase may alternatively be, for example, SGK, PKB or p70 S6 kinase. It is particularly preferred that the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala. The mutated protein kinase may be useful in determining whether a polypeptide or compound interacts with the hydrophobic (PIF binding) pocket or phosphate binding pocket of the unmutated protein kinase. For example, the abilities of a compound (including polypeptide) to bind to the mutated and unmutated protein kinase, or to modulate the activity of the protein kinase towards one or more substrates of the protein kinase, may be measured and compared.

The mutated protein kinase may alternatively or in addition be mutated at a residue forming part of the "hydroxyl-pocket" discussed in Example 6, for example the residue equivalent to Thr222 and/or Gln 220 of full length human PDK1. These residues are involved in the binding of the UCN-01 7-hydroxyl group.

A further aspect of the invention provides a polynucleotide encoding a mutated protein kinase of the invention. A still further aspect of the invention provides a recombinant polynucleotide suitable for expressing a mutated protein kinase of the invention. A yet further aspect of the invention provides a host cell comprising a polynucleotide of the invention.

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A further aspect of the invention provides a method of making a mutated protein kinase of the invention, the method comprising culturing a host cell of the invention which expresses said mutated protein kinase and isolating said mutated protein kinase.

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A further aspect of the invention provides a mutated protein kinase obtainable by the above method.

Examples of these aspects of the invention are provided in Example 1, and may be prepared using routine methods by those skilled in the art, for example as described in WO 00/35946.

For example, the above mutated protein kinase may be made by methods well known in the art and as described below and in Example 1 or 2, for example using molecular biology methods or automated chemical peptide synthesis methods.

It will be appreciated that peptidomimetic compounds may also be useful. Thus, by "polypeptide" or "peptide" we include not only molecules in which amino acid residues are joined by peptide (-CO-NH-) linkages but also molecules in which the peptide bond is reversed. Such retro-inverso peptidomimetics may be made using methods known in the art, for example such as those described in Mézière et al (1997) J. Immunol. 159, 3230-3237, incorporated herein by reference. This approach involves making pseudopeptides containing changes involving the backbone, and not the orientation of side chains. Retro-inverse peptides, which contain NH-CO bonds instead of CO-NH peptide bonds, are much more resistant to proteolysis.

Similarly, the peptide bond may be dispensed with altogether provided that an appropriate linker moiety which retains the spacing between the Cα atoms of the amino acid residues is used; it is particularly preferred if the linker moiety has substantially the same charge distribution and substantially the same planarity as a peptide bond.

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It will be appreciated that the peptide may conveniently be blocked at its N-or C-terminus so as to help reduce susceptibility to exoproteolytic digestion.

The invention further provides a method of identifying a compound that modulates the protein kinase activity of a protein kinase having a hydrophobic pocket and phosphate binding pocket in the positions equivalent to the hydrophobic (PIF binding) pocket and phosphate binding pocket of PDK1, as defined above (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to the said mutated protein kinase of the invention.

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The method may further comprise determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated at the said residue. When the protein kinase is PDK1, it may lack a functional PH domain (ie it may lack a PH domain capable of binding a phosphoinositide).

It will be appreciated that the protein kinase or mutated protein kinase may be a fusion protein comprising a tag, for example to aid purification, for example a GST tag, as described in Example 1.

The capability of the said PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) polypeptide with regard to interacting with or binding to a polypeptide or other compound may be measured by any method of detecting/measuring a protein/protein interaction or other compound/protein interaction, as discussed further below. Suitable methods include methods analagous to those described in Example 1, as well as other methods, for example yeast two-hybrid interactions, co-purification, ELISA, co-immunoprecipitation and surface plasmon resonance methods. Thus, the said PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may be considered

capable of binding to or interacting with a polypeptide or other compound if an interaction may be detected between the said PDK1 polypeptide and the said interacting polypeptide by ELISA, co-immunoprecipitation or surface plasmon resonance methods or by a yeast two-hybrid interaction or copurification method, for example as described in Example 1.

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It is preferred that the interaction can be detected using a surface plasmon resonance method, as described in Example 1. The interacting polypeptide (for example a polypeptide comprising a phosphorylated "hydrophobic motif", for example S6K-pHM; see example 1) may be immobilised on the test surface, for example it can be coupled through amino groups to a SensorChip CM5TM, according to the manufacturer's instructions, or a biotinylated polypeptide can be bound to an avidin coated SensorChip SA. The protein kinase (at concentrations between, for example 0 and between 10μM and 1.0μM, for example 2μM) is then injected over the surface and steady state binding determined in each case. From these measurements a K_d can be determined. It is preferred that the interaction has a K_d of less than 8µM, more preferably less than 5µM, 2µM, 1µM, 500nM, 300nM, 200nM or 100nM, for example about 150nM. Alternatively, a K_d can be determined for a polypeptide or other compound in competition with the immobilised polypeptide (or other compound). The protein kinase (for example at a concentration of 0.5 µM) is mixed with free polypeptide (for example, at concentrations between 0 and 3µM) and the mixture injected over the immobilised polypeptides. The steady state binding is determined in each case, from which the K_d of the interaction can be determined using the Cheng-Prescott relationship. Alternatively, the interaction may be expressed in terms of an observed response or relative observed responses, measured in terms of mass of protein bound to the surface, as described in Example 2. For example, the polypeptide may be immobilised by amino coupling to a SensorChip CM5 and each protein kinase (for example different mutated protein kinases, as discussed below) for example at a concentration of 1.0µM or a range of concentrations, injected over the immobilised polypeptide. Alternatively, the polypeptide may be immobilised on a SA SensorChip and each protein kinase, for example at a concentration of 40nM or a range of concentrations injected over the immobilised polypeptide. The steady state response for each protein kinase is determined, for example expressed in Response Units (RU). 1000RU corresponds to 1 ng/mm² of protein bound to the surface. A response of less than 10RU may indicate that no interaction has taken place. A response of at least 10RU may indicate that the immobilised and injected molecules interact with each other.

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It will be appreciated that the above methods may be used to determine whether a particular polypeptide or compound interacts with a protein kinase or mutated protein kinase.

The effect of the compound on the rate or degree of phosphorylation of a hydrophobic pocket and/or phosphate binding pocket-dependent substrate may be determined. A compound may be selected that decreases the protein kinase activity of the said protein kinase, for example PDK1, towards a hydrophobic pocket-dependent substrate or a phosphate binding pocket-dependent substrate and does not affect or increases the protein kinase activity towards a hydrophobic pocket or phosphate binding pocket-independent substrate, for example PKB when the kinase is PDK1. An activator of PDK1 may mimic insulin and may be useful in treating diabetes or obesity, and may protect cells from apoptosis.

Compounds that bind specifically to the phosphate binding site may activate PDK1 (or other AGK kinase having a phosphate binding site). Also

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compounds that bind to the residues forming part of the pohsphate binding site might transduce the negative effect and inhibit the kinase activity. A compound interacting with the phosphate binding site of PDK1 may be an activator, but only of a subset of substrates. Some substrates of PDK1 require the interaction with the phosphate binding site, such as S6K and SGK.

To generate a specific molecule that could bind to the phosphate and/or PIF-binding pocket of PDK1 a anti-idiotype strategy using combinatorial RNA libraries could be employed. Previous studies have established that Combinatorial RNA libraries can be used to isolate specific ligands, called aptamers, for virtually any target molecule by a procedure probably best known as SELEX (Ellington, A. D., and Szostak, J. W. (1990) Nature 346, 818-822; Tuerk, C., and Gold, L. (1990) Science 249, 505-510). Using this approach RNA molecules that interact with antibodies raised against PIFtide or peptides that encompass the hydrophobic motif of AGC kinases which are phosphorylated at their hydrophobic motif would be selected (preferably antibodies that are specific for the phosphorylated form ie bind the phosphorylated form but not the non-phosphorylated form). These RNA species then may have the intrinsic conformation to interact with the phosphate binding (and possibly also the PIF-binding) pocket(s) of PDK1.

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Antibodies to the phosphate binding pocket may be produced. For example, animals could be immunised with wild type PDK1. Serum could then be purified with a column where the resin is coated with wild type PDK1 used for the immunisation. Specific antibodies could then be passed through columns coated with mutant PDK1 molecules differing only in that they have specific mutations in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala. Antibodies that don't bind to this mutant will either be specific antibodies that recognise the specific

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motifs or antibodies that are sensitive to the conformational changes associated with these mutations. The opposite development could also be performed: antibodies against a mutant PDK1 having a specific mutation(s) in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala, could be produced and the serum further purified through columns coated with wild type PDK1.

Thus, a further aspect of the invention provides an antibody reactive with the phosphate binding pocket of PDK1 or other hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150. A further aspect of the invention provides an antibody reactive with PDK1 or other phosphate-binding pocket-containing protein kinase as defined above but not with the said protein kinase mutated at the phosphate binding site, or vice versa. A further aspect of the invention provides a method for preparing or selecting an antibody wherein the antibody is prepared or selected against a said protein kinase (for example PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.

25 By the term "antibody" is included synthetic antibodies and fragments and variants (for example as discussed above) of whole antibodies which retain the antigen binding site. The antibody may be a monoclonal antibody, but may also be a polyclonal antibody preparation, a part or parts thereof (for example an F_{ab} fragment or F(ab')₂) or a synthetic antibody or part thereof.

30 Fab, Fv, ScFv and dAb antibody fragments can all be expressed in and

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secreted from *E. coli*, thus allowing the facile production of large amounts of the said fragments. By "ScFv molecules" is meant molecules wherein the V_H and V_L partner domains are linked via a flexible oligopeptide. IgG class antibodies are preferred.

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Suitable monoclonal antibodies to selected antigens may be prepared by known techniques, for example those disclosed in "Monoclonal Antibodies: A manual of techniques", H. Zola (CRC Press, 1988) and in "Monoclonal Hybridoma Antibodies: techniques and Applications", JGR Hurrell (CRC Press, 1982), modified as indicated above. Bispecific antibodies may be prepared by cell fusion, by reassociation of monovalent fragments or by chemical cross-linking of whole antibodies. Methods for preparing bispecific antibodies are disclosed in Corvalen *et al*, (1987) *Cancer Immunol. Immunother.* 24, 127-132 and 133-137 and 138-143.

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A general review of the techniques involved in the synthesis of antibody fragments which retain their specific binding sites is to be found in Winter & Milstein (1991) *Nature* **349**, 293-299.

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For example, an antibody that does not bind PDK1 Arg131Ala could be specifically recognising this residue in the phosphate binding site, but could also be recognising specifically the inactive conformation of PDK1, which is stabilised by Arg 131. The opposite development could also be performed: antibodies against a mutant PDK1 Arg131Ala could be produced and the serum further purified through columns coated with wild type PDK1. In this way, antibodies may be prepared that would either not be able to interact with the phosphate binding site Arg 131 but only when a small residue is in its place, or antibodies that are probes for the active conformation of PDK1. These conformational probes could be used in high throughoutput screenings, HTS, in the search of compounds that are capable

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of modifying the conformation of the given protein kinase. Antibodies could have been produced with previous knowledge to detect active protein kinases by immunising with active protein kinases, but in those cases, the antibodies would have recognised also the phosphorylation events that make a protein kinase be active. In the methodology here described using the conformational probes could be easily isolated. antibodies, Furthermore, antibodies obtained from an active protein kinase (with overall modifications that make it active) could be further purified through a column coated with the inactive protein kinase (keeping the non bound fraction) and then further purifyied on a column coated with a protein kinase consisting of an activating mutation (such as R131A in the case of PDK1), retaining the specifically bound fraction, which could be an active conformation probe. This type of approach could also allow the development of conformation specific probes by the use of activating or inhibiting mutations.

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A further aspect of the invention provides a kit of parts useful in carrying out a method according to the preceding aspect of the invention, comprising (1) a mutated protein kinase of the invention and (2) the protein kinase which is not a mutated said protein kinase as defined above.

The protein structures described herein (for example with the co-ordinates shown in Examples 2, 3 or 4, or structures modelled thereon) may be useful in designing further reagents that may be useful in drug screening assays or characterisation of protein kinase activity or regulation. For example, such structures may be useful in designing mutants that may be useful in FRET-based activities, for example in which surface residues near to binding sites are mutated to cysteines to allow coupling of chromophores. For example, the cysteine residue may be fluorescently-labelled, and a change in

fluorescence intensity or frequency may be detected in an assay. Any thiol-reactive fluorophore, for example BADAN (see, for example, Wadum et al Fluorescently labeled bovine acyl-CoA binding protein — an acyl-CoA sensor. Interaction with CoA and acyl-CoA esters and its use in measuring free acyl CoA esters and non-esterified fatty acids (NEFA); Hammarstrom et al (2001) Biophys J 80(6), 2867-2885; Schindel et al (2001) Eur J Biochem 268(3), 800-808), could be used to label the cysteine. An alternative suitable fluorophore is Acrylodan (Richieri et al (1992) J Biol Chem 267(33), 23495-23501).

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It will be appreciated that the invention provides screening assays for drugs which may be useful in modulating, for example either enhancing or inhibiting, the protein kinase activity of a protein kinase (for example, the protein kinase activity towards a particular substrate) having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of Protein Kinase A (PKA) that is defined by residues including Lys76, Leu116, Val80 and/or Lys111 of full-length mouse PKA, for example PDK1, SGK, PKB, PKA or p70 S6 kinase, for example the PDK1 or PDK2 activity (as discussed above) of PDK1. The compounds identified in the methods may themselves be useful as a drug or they may represent lead compounds for the design and synthesis of more efficacious compounds.

The compound may be a drug-like compound or lead compound for the development of a drug-like compound for each of the above methods of identifying a compound. It will be appreciated that the said methods may be useful as screening assays in the development of pharmaceutical compounds or drugs, as well known to those skilled in the art.

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The term "drug-like compound" is well known to those skilled in the art, and may include the meaning of a compound that has characteristics that may make it suitable for use in medicine, for example as the active ingredient in a medicament. Thus, for example, a drug-like compound may be a molecule that may be synthesised by the techniques of organic chemistry, less preferably by techniques of molecular biology or biochemistry, and is preferably a small molecule, which may be of less than 5000 daltons. A drug-like compound may additionally exhibit features of selective interaction with a particular protein or proteins and be bioavailable and/or able to penetrate cellular membranes, but it will be appreciated that these features are not essential.

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The term "lead compound" is similarly well known to those skilled in the art, and may include the meaning that the compound, whilst not itself suitable for use as a drug (for example because it is only weakly potent against its intended target, non-selective in its action, unstable, difficult to synthesise or has poor bioavailability) may provide a starting-point for the design of other compounds that may have more desirable characteristics.

20 It is appreciated that screening assays which are capable of high throughput operation are particularly preferred. Examples may include cell based assays and protein-protein binding assays. An SPA-based (Scintillation Proximity Assay; Amersham International) system may be used. For example, beads comprising scintillant and a substrate polypeptide or interacting polypeptide may be prepared. The beads may be mixed with a sample comprising ³²P- or ³³P-γ-labelled PDK1 or other protein kinase or mutated protein kinase (as defined above) and with the test compound. Conveniently this is done in a 96-well or 384-well format. The plate is then counted using a suitable scintillation counter, using known parameters for ³²P or ³³P SPA assays. Only ³²P or ³³P that is in proximity to the scintillant,

i.e. only that bound to the substrate or interacting polypeptide that is bound to the beads, is detected. Variants of such an assay, for example in which the substrate or interacting polypeptide is immobilised on the scintillant beads *via* binding to an antibody or antibody fragment, may also be used.

- It will be understood that it will be desirable to identify compounds that may modulate the activity of the protein kinase in vivo. Thus it will be understood that reagents and conditions used in the method may be chosen such that the interactions between, for example, the said protein kinase and the interacting polypeptide, are substantially the same as between the human protein kinase and a naturally occurring interacting polypeptide comprising the said amino acid sequence. It will be appreciated that the compound may bind to the protein kinase, or may bind to the interacting polypeptide.
- The compounds that are tested in the screening methods of the assay or in other assays in which the ability of a compound to modulate the protein kinase activity of a protein kinase, for example a hydrophobic pocket-containing protein kinase, as defined above, may be measured, may be compounds that have been selected and/or designed (including modified) using molecular modelling techniques, for example using computer techniques.

A further aspect of the invention is a compound identified or identifiable by the above selection/design methods of the invention, for example an RNA molecule or antibody identifiable as defined above.

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A still further aspect of the invention is a compound (or polypeptide or polynucleotide) of the invention or identified or identifiable by the above selection/design methods of the invention, for use in medicine. Conditions

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or diseases in which such compounds, polypeptides or polynucleotides may be useful are indicated below.

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The compound (or polypeptide or polynucleotide) may be administered in any suitable way, usually parenterally, for example intravenously, intraperitoneally or intravesically, in standard sterile, non-pyrogenic formulations of diluents and carriers. The compound (or polypeptide or polynucleotide) may also be administered topically, which may be of particular benefit for treatment of surface wounds. The compound (or polypeptide or polynucleotide) may also be administered in a localised manner, for example by injection. The compound may be useful as an antifungal (or other parasitic, pathogenic or potentially parasitic or pathogenic organism) agent.

A further aspect of the invention is the use of a compound (or polypeptide 15 or polynucleotide) as defined above in the manufacture of a medicament for the treatment of a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket, as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin PDK1/PDK2/SGK/PKB/p70 and/or signalling pathway 20 kinase/PRK2/PKC signalling. The patient may be in need of inhibition of a said hydrophobic/phosphate binding pocket-containing kinase in an infecting organism, for example the patient may have a fungal infection for which treatment is required. The compound may inhibit the infecting organism's (for example fungal) hydrophobic/phosphate binding pocket-25 containing protein kinase, but may not inhibit the patient's equivalent hydrophobic/phosphate binding pocket-containing protein kinase.

A further aspect of the invention is a method of treating a patient in need of modulation of signalling by a protein kinase having a

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hydrophobic/phosphate binding pocket as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound (or polypeptide or polynucleotide) as defined above.

A compound that is capable of reducing the activity of PKC, for example PKCβ, PRK1 or 2, PDK1 (ie the PDK1 and/or the PDK2 activity), PKB, SGK or p70 S6 kinase may be useful in treating cancer. PDK1, for example via PKB and/or SGK, may be capable of providing a survival signal that protects cells from apoptosis induced in a variety of ways (reviewed in Cross et al (1995) Nature 378, 785-789 and Alessi & Cohen (1998) Curr. Opin. Genetics. Develop. 8, 55-62). Thus, such compounds may aid apoptosis. Reduction of the activity of PDK1, PKB, SGK and/or p70 S6 kinase may promote apoptosis and may therefore be useful in treating cancer. Conditions in which aiding apoptosis may be of benefit may also include resolution of inflammation.

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A compound is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase may be useful in treating diabetes or obesity, or may be useful in inhibiting apoptosis. Increased activity of PDK1, PKB, SGK or p70 S6 kinase may lead to increased levels of leptin, as discussed above, which may lead to weight loss; thus such compounds may lead to weight loss. For example, such compounds may suppress apoptosis, which may aid cell survival during or following cell damaging processes. It is believed that such compounds are useful in treating disease in which apoptosis is involved. Examples of such diseases include, but are not limited to, mechanical (including heat) tissue injury or ischaemic disease, for example stroke and myocardial infarction, neural injury and myocardial infarction. Thus the patient in need of modulation of the activity of PDK1, PKB, SGK

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or p70 S6 kinase may be a patient with cancer or with diabetes, or a patient in need of inhibition of apoptosis, for example a patient suffering from tissue injury or ischaemic injury, including stroke.

- Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identified or identifiable by the screening methods of the invention.
- A still further invention provides a use of a compound identifiable by the screening methods of the invention in the manufacture of a medicament for treating an ischaemic disease in a patient.
- Thus, a further aspect of the invention provides a method of treating a

 patient with an ischaemic disease the method comprising administering to
 the patient an effective amount of a compound identifiable by the screening
 methods of the invention.
- If the patient is a patient in need of promotion of apoptosis, for example a patient with cancer, it is preferred that the compound of the invention that is used in the preparation of the medicament is capable of reducing the activity of PDK1, PKB, SGK or p70 S6 kinase. If the patient is a patient with diabetes or a patient in need of inhibition of apoptosis, for example a patient with ischaemic disease, it is preferred that the compound of the invention that is used in the preparation of the medicament is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase.

All documents referred to herein are hereby incorporated by reference.

The invention is now described in more detail by reference to the following, non-limiting, Figures and Examples.

Figure legends

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1. Overview of the PDK1 structure.

The PDK1 kinase domain backbone is shown in a ribbon representation, with the secondary structure elements for residues 74-163 in the lower half of the Figure and for residues 164- 358 in the upper part of the Figure. Helix αG , encompassing residues 287-295 (which makes a crystal contact to a symmetry related PDK1 molecule, Fig. 2), is at the bottom right of the Figure. Key residues discussed in the text are shown as a sticks model. ATP is shown as a sticks model. A simulated annealing |Fo -|Fc', ϕ calc map is shown in black, contoured at 3 σ . The phosphoserine and the sulphate discussed in the text are also shown.

2. The PIF-pocket

A. A surface representation of the putative PIF binding pocket is shown and compared to the pocket interacting with the C-terminal FXXF motif in PKA. For PDK1, the αG helix of a symmetry-related molecule is shown as a ribbon, in PKA the C-terminus is also shown as a ribbon. Aromatic amino acids buried in the pocket are shown as sticks; further side chains interacting with the pocket are also shown as sticks. Helix αC is also shown as a ribbon in both PDK1 and PKA (at bottom of images). In PDK1, the ordered sulphate ion and basic residues interacting with it are also shown.

B. A stereo image of the residues lining the PIF-pocket is shown. The PDK1 backbone is shown as a grey ribbon. Side chains are shown as sticks. Hydrogen bonds to the sulphate ion are shown as black dotted lines.

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3. Structure-based sequence alignment

The sequences of PKA and PDK1 are aligned according to a structural superposition performed in WHAT IF [Vriend, 1990]. Sequence numbering is according to PDK1. β -strands (arrows) and α -helices (bars) are shown for the PDK1 structure according to a DSSP [Kabsch and Sander, 1983] secondary structure assignment, and labelled consistent with the secondary structure element names proposed for PKA [Taylor and Radzioandzelm, 1994]. Residues lining the PIF-pocket are indicated with a black dot. Residues hydrogen bonding the sulphate ion are indicated by arrows. The PDK1 residues equivalent to Ser53 and Gly186 in PKA, are labelled with an asterisk.

4. PDK1 binding & activation studies

- Binding and activation of wild type and mutant forms of PDK1 to a phosphopeptide derived from the hydrophobic motif of S6K1. The binding of the wild type (wt) PDK1 and indicated mutants to a phosphopeptide comprising the hydrophobic motif of S6K1 (S6K-pHM: SESANQVFLGFT*YVAPSV, where T* indicates phospho-threonine) was analysed by surface plasmon resonance as described in the Materials and Methods.
 - A. The sensor chip SA was coated with 12RUs of the biotinylated S6K-pHM peptide and the binding was analysed following injection of 270 nM wild type PDK1, PDK1 [T148A] and PDK1 [K76A]. No detectable binding to S6K-pHM was observed using PDK1 [R131A] or PDK1 [Q150] (data not shown).
 - **B.** As in **A.** except that binding was analysed over a range of PDK1 concentrations (2-2150nM). The response level at the steady state binding is plotted versus the log of the PDK1 concentration. The estimated Kd was

obtained by fitting the data to a sigmoid curve using Kaleidagraph software. Kd for wild type PDK1 was 642 – 131 nM, PDK1 [T148A] was 64 – 7 nM and PDK1 [K76A] was 1744 – 167 nM. No detectable binding of PDK1 to the non-phosphorylated S6K-HM peptide (SESANQVFLGFTYVAPSV) was detected with wild type PDK1 or any of the mutants (data not shown). C. Activation of the indicated forms of PDK1 by S6K-pHM and S6K-HM. PDK1 activity was measured using the peptide substrate (T308tide) in the presence of the indicated concentrations of S6K-pHM (closed circles) and S6K-HM (open circles) as described in the methods. Assays were performed in triplicate and similar results obtained in 2 separate experiments. The results are the average – SD for a single experiment.

5. Interactions of regulatory phosphates with the αC helix

- A. The PDK1 backbone is shown as a ribbon, with helix α C in the centre of the view. Key residues are shown as sticks. The sulphate ion and the phosphate on the activation loop are also shown. A sticks model of ATP is shown. Hydrogen bonds are shown as black dotted lines.
 - B. Alignment of the amino acid sequence forming part of the phosphate pocket on PDK1 with the equivalent region of the indicated AGC kinases. Identical residues are denoted by white letters on a black background and
 - similar residues by gray boxes. Arrows indicate the residues corresponding to Lys 76, Arg131, Thr148 and Gln150 of PDK1.

6. Essential dynamics

- A. Projection of all available PKA crystal structures (labelled dots) and the PDK1 structure (diamond) onto the first two eigenvectors (i.e. the ones with the two largest eigenvalues) calculated from the PKA structures.
 - B. Graphic representation of the motion along the first eigenvector, generated by projecting two structures at -4 nm (black) and +4 nm (grey).

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7. Alignment of AGC protein kinase family members.

8. Staurosporine and UCN-01 electron density.

The staurosporine and UCN-01 molecules are shown in a stick representation. Hydrogen bonding atoms (Table 4) are labelled according to [49]. The unbiased $|F_o|-|F_c|$, ϕ_{calc} maps are contoured at 2.5 σ .

9.. Details of the inhibitor binding sites.

The bridging water molecule is shown as a sphere. Hydrogen bonds are indicated by black dotted lines. Labelled residues hydrogen-bond the inhibitor molecules.

Example 1: High resolution crystal structure of the human PDK1 catalytic domain defines the regulatory phosphopeptide docking site

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) plays a key 15 role in insulin/growth factor induced signalling pathways through phosphorylation of downstream AGC-kinases such as Protein Kinase B/Akt and p70 ribosomal S6 kinase (S6K1). Here we describe the 2.0 Å crystal structure of the PDK1 kinase domain in complex with ATP. The structure defines the hydrophobic pocket termed the 'PIF-pocket'which plays a key 20 role in mediating the interaction and phosphorylation of certain substrates such as S6K1. In the PDK1 structure, this pocket is occupied by an extensive crystallographic contact with another molecule of PDK1, reminiscent of the interaction of Protein Kinase A with the hydrophobic motif at its C-terminus. Previous studies have shown that phosphorylation 25 of S6K1 at its C-terminal PIF-pocket-interacting motif, promotes the binding of S6K1 with PDK1, suggesting that there may be a phosphate docking site located nearby the PIF-pocket. Interestingly, close to the PIFpocket on the PDK1 structure, there is an ordered sulphate ion, interacting tightly with four surrounding side chains. The roles of these residues were 30

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investigated through a combination of site directed mutagenesis and kinetic studies, the results of which suggest that this region of PDK1 does indeed represent a phosphate dependent docking site. An analogous phosphate binding regulatory motif may participate in the activation of other AGC kinases.

Results & Discussion

Overall structure

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The structure of the catalytic domain of PDK1 was solved by molecular replacement and refined to an R-factor of 0.19 (Rfree=0.22). PDK1 assumes the classic bilobal kinase fold (Fig. 1) and is similar to the only other AGC kinase structure solved, that of PKA (RMSD.of 1.0 Å on C α atoms with PDB entry 1STC [Prade et al., 1997]). The form of PDK1 that was crystallized comprised residues 51 to 359. The tip of the activation loop (residues 233-236) is disordered, as observed in other kinase structures [Johnson et al., 1996]. The N-terminus (residue 51-70), which is pointing into a large void generated by the crystallographic symmetry, is also disordered. In contrast, the N-terminal extension to the kinase domain of PKA assumes an amphipathic a -helix (termed \alpha A-helix), and packs against the kinase core [Knighton et al., 1991]. The cluster of hydrophobic residues that mediates this interaction in PKA is not present in PDK1, suggesting that the N-terminus of PDK1 could have a different function from that of PKA. Interestingly, it has recently been shown that the N-terminus of PDK1 (residues 1-50) interacts with Ral guanine nucleotide exchange factors [Tian et al., 2002]. Thus, this region may assume a unique conformation in PDK1, which is not defined by the structure described here.

PDK1 was crystallised in the presence of ATP but in the absence of any divalent cations. In the early stages of the refinement well-defined density

for the entire ATP molecule could be observed. ATP adopts a different conformation to that observed in other kinase-ATP complexes (Fig. 1). Perhaps due to the absence of divalent cations, the generally observed kink between the β and γ phosphate caused by the interaction with such an ion, is not seen in the PDK1 structure.

It is known that PDK1 can phosphorylate itself on residue Ser 241 in the activation loop and that this phosphorylation is required for PDK1 activity [Alessi et al., 1997]. Indeed, we observed density for a phosphate attached to this residue (Fig. 1), and extensive interactions are observed between this phosphoserine and residues from the C-terminal lobe and α C-helix (Fig. 1). The interaction between Ser241 and the C-terminal lobe is similar to the equivalent interactions in PKA but as discussed below the binding to the α C-helix differs.

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The PIF-pocket

As outlined in the introduction, PDK1 was postulated to possess a pocket (the 'PIF-pocket') in the small lobe of its catalytic domain, required for the binding of PDK1 to the hydrophobic motif of its substrates [Biondi et al., 2000]. The PDK1 structure described here indeed reveals such a pocket, and shows that it lies in a location similar to the FXXF-binding pocket in PKA (Fig. 2). PDK1 residues Lys115, Ile118, Ile119 on the α B helix (Fig. 2), Val124, Val127 on the α C helix and Leu155 on β -sheet 5 form an approximately 5 Å deep pocket. Previous work has shown that mutation of Leu 155 to Glu abolishes the ability of PDK1 to interact with a peptide that encompasses the hydrophobic motif of PRK2 (PIFtide) [Biondi et al., 2000] as well as with S6K1, SGK1, PKC ζ and PRK2 [Balendran et al., 2000, Biondi et al., 2000]. In addition, mutation of Lys115, Ile119, Glu150, and

Leu155 to alanine, reduced the affinity of PDK1 for PIFtide approximately 10-fold, but did not affect the ability to phosphorylate and activate S6K1 and SGK1 [Biondi et al., 2001]. These results are in agreement with the crystal structure of the PIF-pocket, since Leu155 is located at the center and the other residues line the wall of the pocket (Fig. 2). Interestingly, in our structure, the PIF-pocket is occupied by helix αG of a symmetry related molecule (Fig. 2). Tyr288 and Phe291 make hydrophobic contacts in this pocket with almost all pocket-lining residues, remarkably reminiscent of the interactions of the phenylalanines in the FXXF motif in PKA and their hydrophobic docking site in the equivalent region of the kinase domain (Fig. 2). In addition, residues Glu287, Gln292, Ile295 and Lys296 on the symmetry related loop also form contacts with residues lining the PIFpocket. In total, 244 ² Å of accessible surface is buried by this contact, suggesting this is a tight interaction. However, the significance of this interaction is not clear as an oligomerisation event for PDK1 has not been demonstrated in solution previously. Indeed both the isolated catalytic domain of PDK1 that was crystallised and full length PDK1 migrate in gel filtration chromatography as apparent monomeric species (data not shown).

20 The phosphate pocket

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As outlined in the introduction, substrates of PDK1, such as S6K1, interact with the PIF-pocket of PDK1 with higher affinity when they are phosphorylated at their hydrophobic motif. This suggested that a regulatory phosphate binding site may be located close to the PIF-pocket. During refinement of the PDK1 structure, it became clear that next to the PIF-pocket another small pocket was present, occupied by a tetrahedral oxyanion (Fig. 2). As 2.0 M of sulphate was present in the crystallisation conditions, this was assigned as a sulphate ion. The ion interacts with four

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residues lining the pocket, namely Lys76, Arg131, Thr148 and Gln150. Because of its close proximity to the PIF-pocket (approximately 5Å) it is possible that this sulphate-occupied pocket could represent the binding site for the phosphate on the phosphopeptide. To investigate this further, we mutated Lys76, Arg131, Thr148 and Gln150 to Ala, in order to verify the contribution of each of these residues in enabling PDK1 to interact with a peptide encompassing the hydrophobic motif of S6K1, in which the residue equivalent to Thr412 was phosphorylated (termed S6K-pHM). A quantitative surface plasmon resonance based binding assay (Fig. 4A) showed that wild type PDK1 interacted with S6K-pHM, with a Kd of 0.6 µM with S6K-pHM but not detectably to the non-phosphorylated form of this peptide (S6K-HM). The PDK1[R131A] and PDK1[Q150A] mutants did not detectably interact with S6K-pHM in this assay (Fig. 4B), confirming that the interactions these residues make in the PDK1 structure are of key importance. The PDK1[K76A] mutant interacted with 3-fold lower affinity (Kd 1.7 µM) with S6K-pHM. The PDK1[T148A] mutant however possessed about 10-fold higher (Kd 0.06 µM) affinity for S6KpHM than wild type PDK1. Moreover, the dissociation of PDK1[T148A] from S6K-pHM is markedly slower than that of wild type PDK1 or PDK1[K76A] (Fig 4A). These findings are unexpected as Thr148 is within hydrogen bonding distance of the sulphate (Fig. 2), but indicate that this residue may play a role in enabling the dissociation of PDK1 from S6KpHM.

The binding of PDK1 to PIFtide stimulates up to 4-fold the rate at which PDK1 phosphorylates a small peptide that encompasses the activation loop motif of PKB (termed T308tide) [Biondi et al., 2000], indicating that occupancy of the PIF-pocket of PDK1 activates the enzyme. Similarly, the binding of a phosphopeptide corresponding to the hydrophobic motif of RSK stimulated PDK1 activity 6-fold [Frodin et al., 2000]. We have now

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also found that the binding of S6K-pHM to wild type PDK1 induces a maximal 5-fold activation, with a half maximal activation occurring at a concentration of approximately 50 µM S6K-pHM (Fig. 4C). We next assayed the specific activities of PDK1[K76A], PDK1[R131A], PDK1[T148A] and PDK1[Q150A] mutants in the absence and presence of increasing concentrations of S6K-pHM (Fig. 4C). The PDK1[K76A] possessed the same specific activity towards T308tide in the absence of S6K-pHM as wild type PDK1, but an approximately 3-fold higher concentration of S6K-pHM was required to half maximally activate PDK1[K76A], consistent with the reduced affinity of this form of PDK1 for S6K-pHM (Fig. 4A,B). The PDK1[R131A] mutant possessed a 3-fold higher specific activity towards Thr308tide in the absence of S6K-pHM (Fig. 4C), as has been observed previously with certain other PIF-pocket mutants of PDK1(PDK1[K115A] and PDK1[L155E]) [Biondi et al., 2000]. However, in accordance with the inability of PDK1[R131A] to bind S6KpHM in the Biacore assay (Fig. 4B), it was not significantly activated by concentrations of S6K-pHM below 0.1 mM and its activity was only moderately further increased by the addition of high concentrations (0.3 and 1 mM) of S6K-pHM (Fig. 4C). The activity of a mutant of PDK1 in which both Lys76 and Arg131 were changed to Ala was activated even less significantly by these high concentrations of S6K-pHM. The PDK1[T148A] and PDK1[Q150A] mutants possessed similar specific activity towards T308tide as wild type PDK1 in the absence of S6K-pHM. PDK1[T148A] mutant was activated similarly as wild type PDK1 by S6KpHM and consistent with the inability of PDK1[Q150A] to interact with S6K-pHM, this mutant of PDK1 was not significantly activated by concentrations of S6K-pHM below 0.1 mM but at 0.3 and 1 mM peptide a 2-3 fold activation was observed (Fig. 4).

At very high peptide concentrations (0.3-1 mM) the non-phosphorylated S6K-HM

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peptide induced a small (<2-fold) activation of PDK1 (Fig. 4C). Interestingly, despite the PDK1[K76A] and PDK1[R131A] mutants being markedly less able to interact with the phosphorylated S6K-pHM peptide, than wild type PDK1, high concentrations of the S6K-HM peptide activated PDK1[K76A] and PDK1[R131A] to a similar extent as wild type PDK1, indicating that the ability of these mutants to interact weakly with the S6K-HM peptide was not affected.

We evaluated the sequence conservation in the phosphate pocket of the insulin/growth factor-activated AGC family kinases (PKBa, S6K1, SGK1 and RSK1). Sequence alignments indicate that this pocket is conserved amongst these kinases (Fig 5A). The most conserved residue is Gln150 which is found in all of these AGC kinases and the residue equivalent to Lys76 is always a basic residue (Fig. 5A). Arg131 is conserved in S6K1, SGK1 and RSK1 but not in PKB α , or PKB β or PKB γ , where it is an Asn or Ser. Thr148 is conserved in PKBa and SGK1 but is an Ala in S6K1 and RSK1. Interestingly, we have found the Thr 148Ala mutation in PDK1 did not disrupt the phosphate pocket (Fig 4). As PKBa, S6K1, SGK1 and RSK1 require to be phosphorylated at their hydrophobic motif to be maximally activated, it is tempting to speculate that the C-terminal hydrophobic motifs of these enzymes, when phosphorylated, bind to their own PIF/phosphate pockets, thereby generating a network of interactions similar to that of PDK1. In support of this, PKBa, S6K1, SGK1 and RSK1 also require phosphorylation of their activation loop at the position equivalent to Ser241 for activity. Consistent with PKA not possessing a phosphate pocket, Lys76 and Gln150 are not conserved in PKA (Fig. 3), and indeed such a pocket is not observed in the PKA structure (Fig. 2).

The αC helix

The PDK1 structure shows that, as in other protein kinases [Johnson et al., 2001, Husen and Kuriyan, 2002], the α C helix (residues 124-136) is a key signal integration motif in the kinase core. One turn of the PDK1 α C helix (residues 129-131, Figs. 3, 5) links together the N-terminal lobe, the C-terminal lobe and the active site. Arg129 points towards the activation loop and forms two hydrogen bonds with the phosphorylated Ser241, whereas Arg131 forms two hydrogen bonds with the sulphate in the phosphate pocket (Fig. 5). Glu130 coordinates Lys111 which forms a hydrogen bond with the α -phosphate of the bound ATP. This interaction is conserved in all protein kinases and shown to be crucial for activation [Johnson et al., 2001, Husen and Kuriyan, 2002]. An additional residue, His126, forms a third hydrogen bond with the phosphorylated Ser241. Val124 and Val127 on the α C helix are involved in formation of the PIF-pocket (Fig. 5).

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The αC helix provides a structural link between the putative phosphopeptide binding pocket and the phosphoserine in the activation loop. The fact that R131A has higher basal activity than wild type PDK1 may indicate that this residue plays tuning role in the PDK1 structure, not only participating in the activation of PDK1 in the presence of a phosphate ion, but also on keeping the equilibrium of the enzyme towards an inactive conformation in the absence of S6K-pHM. To our knowledge this is the first report of a kinase structure in which the αC helix is positioned by 2 regulatory phosphate binding sites on either side of the helix (Fig 5). This provides a possible sensor-mechanism for linking the phosphorylation-state of the activation loop and the phosphopeptide binding event in the PIF-pocket to PDK1 activity.

Activation state

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All structures of PKA solved to date show a phosphorylated T-loop and are therefore assumed to be in an active state. In addition to the unphosphorylated versus phosphorylated states of PKA, there appear to be two main conformational states possible for the latter [Zheng et al., 1993, Johnson et al., 2001]. In the active, closed conformation, all residues are positioned to facilitate phosphoryl transfer. In contrast, the inactive, open conformation is seen in absence of a nucleotide, and differs from the closed conformation by conformational changes of the N-terminal and C-terminal domains with respect to each other. In addition, three 'intermediate' structures were described from PKA, having either adenosine (PDB entry 1BKX [Narayana et al., 1997]) or the inhibitors staurosporine (PDB entry 1STC [Prade et al., 1997]) and balanol (PDB entry 1BX6 [Narayana et al., 1999]) in the ATP-binding site. Taylor and colleagues have described a method to distinguish between the active and inactive conformations, based on three distances: His87-pThr197 (αC helix positioning), Ser53-Gly186 (opening of the glycine-rich loop) and Glu170-Tyr330 (C-terminal tail distance to active site) [Johnson et al., 2001]. In PDK1, only one of these distances, the opening state of the glycine rich loop, can be measured due to sequence conservation (Fig. 3). This distance is 12.4 Å, similar to a PKA intermediate conformation (this distance in PKA is 14.2Å for the open, 11.8 Å for intermediate and 10.0 Å for the closed conformation [Johnson et al., 2001]). To allow a more direct comparison of the PDK1 structure with the available PKA structures, we have analysed the conformational state of PDK1 in detail using a novel approach, which involves a principal component analysis (also called "essential dynamics" [Amadei et al.,1993]) of the crystallographic coordinates. In short, this involves the construction of a covariance matrix containing the correlations between atomic shifts (with respect to an average structure) in the ensemble of all available PKA crystal structures. Diagonalisation of this matrix gives eigenvector/eigenvalue sets which describe concerted shifts of atoms

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(eigenvectors) together with the corresponding mean square fluctuation of the structures (eigenvalues). This approach allows a condensed description of PKA conformational states using only a few degrees of freedom, as shown previously for a range of other proteins [van Aalten et al., 1997,van Aalten et al., 2000, de Groot et al., 1998]. Diagonalisation of a covariance matrix built from the backbone atoms of residues 37-196, 198-283 and 286-305 results in a set of eigenvectors that describe concerted motions of the PKA backbone. In Fig. 6A, all PKA structures are projected on a subspace spanned by the first two eigenvectors (i.e. those with the two largest eigenvalues). It appears that the PKA structures cluster in three main areas along the first eigenvector. On the left of the average structure (which by definition has a projection of 0.0 on all eigenvectors) are the structures that are known to be in the "open" conformation (Fig. 6A). Around the average structure lie the structures that have been shown to be in an "intermediate" conformation (complexes with the inhibitors staurosporine, balanol and adenosine). More to the right of the average structure are the PKA structures that are known to be in the "closed" conformation. Thus, we have captured the conformational state of PKA in a single variable, the translation along the first eigenvector. This is further clarified by investigation of the atomic shifts described by this eigenvector in Cartesian space (Fig. 6B). A hinge-bending motion is observed between the Nterminal and C-terminal lobes, opening and closing the active site. It is now possible directly to compare the PDK1 conformational state by projecting the structure (backbone atoms only) onto the PKA eigenvectors. Fig. 6A shows that the conformation of PDK1 is close to the PKA structures that are in an "intermediate" conformation, consistent with the other structural analyses described above.

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Conclusions

We have reported the structure of the PDK1 catalytic domain, which, although similar to PKA, has revealed important features that increase our understanding of the mechanism by which PDK1 is regulated. The structure, together with mutational analyses, defines a phosphopeptide binding pocket, consisting of a separate hydrophobic PIF-pocket and a phosphate binding site, which mediates the interaction of PDK1 with the phosphorylated hydrophobic motif of S6K. This is consistent with the previous hypothesis that phosphorylation of S6K and SGK [Biondi et al., 2001] as well as RSK [Frodin et al., 2000] at their FXXFS/T hydrophobic motif is the trigger for their interaction and phosphorylation by PDK1. In this mechanism the PIF-pocket would physiologically only interact with the Phe residues when the Ser/Thr residue is phosphorylated. Furthermore, as the phosphate pocket is conserved in other AGC kinases, the structural features and network of interaction of the phosphate pocket with the αC helix on PDK1, could provide insight into the mode of activation of other AGC kinases.

Experimental Procedures

Materials

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Mammalian and Insect cells culture reagents were from Life Technologies. SensorChips SA were from BiaCore AB. Glutathione Sepharose, as well as pre- packed HiTrap Q HP and Hiload Superdex 200 prep grade columns were from Amersham Biosciences. Dialysis cassettes were from the Slide-A-Lyzer series (Pierce). Ni-NTA Agarose was from Qiagen. Disposable ultrafiltration devices (polyethersulfone membranes) were from Vivascience. Crystallisation research tools (primary screens, additive

screens and crystallisation plates) were from Hampton Research. Peptides were synthesised by Dr G. Blomberg (University of Bristol, UK).

General methods

Molecular biology techniques were performed using standard protocols. Site directed mutagenesis was performed using a QuickChange kit (Stratagene) following instructions provided by the manufacturer. DNA constructs used for transfection were purified from bacteria using Qiagen plasmid Mega kit according to the manufacturer's protocol, and their sequence verified. Human kidney embryonic 293 cells were cultured on 10 cm diameter dishes in Dulbecco's modified Eagle's medium containing 10% foetal bovine serum.

Buffers

Low Salt Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl; High Salt Buffer: 25mM Tris-HCl pH 7.5, 500 mM NaCl. Lysis Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl 0.07% β -mercaptoethanol, 1mM Benzamidine, and 20 μg/ml PMSF. Buffer A: 50 mM Tris-HCl pH 7.5, 1 mM EGTA, 1 mM EDTA, 1% (by mass) Triton-X 100, 1 mM sodium orthovanadate, 50 mM sodium fluoride, 5 mM sodium pyrophosphate, 0.27 M sucrose, 1 μM microcystin-LR, 0.1% (by vol) β -mercaptoethanol and "complete" proteinase inhibitor cocktail (one tablet per 50 ml, Roche). Buffer B: 50 mM Tris/HCl pH 7.5, 0.1 mM EGTA, 10 mM β -mercaptoethanol and 0.27 M sucrose.

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Expression, purification and characterisation of the kinase domain of PDK1

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A cDNA encoding for human PDK1 amino acid residues 51-359 with a stop codon inserted at position 360, was amplified by PCR reaction using full length human PDK1 cDNA in the pCMV5 vector [Alessi et al., 1997] as a template a 5'primer, which incorporates a BamH1 restriction site, an initiating methionine, a hexahistidine tag.followed by a PreScission protease recognition sequence prior to the residue equivalent to Met51 of PDK1 (ggatcctataaatatggcacatcatcatcatcatctggaagttctgttccaggggcccatggacggcact gcagccgagcctcgg) and the 3' primer applied in this reaction was: 5'ggatcctcaggtgagcttcggaggcgtctgctggtg-3'. The resulting PCR product was ligated into pCR 2.1 TOPO vector (Invitrogen) and then subcloned as a BamH1-BamH1 fragment into pFastbac1 vector (Life Technologies) for baculovirus protein expression. The resulting construct was then used to generate recombinant baculovirus using the Bac-to-Bac system (Life Technologies) following the manufacturer's protocol. The resulting baculoviruses were used to infect Sf21 cells at 1.5 x 106/ml. The infected cells were harvested by centrifugation 72 hours post infection. Cell pellets corresponding to 71 of culture were resuspended in 900 ml of Lysis Buffer and cells lysed in nitrogen cavitation chamber. Cell debris was then pelleted by centrifugation, the supernatant made 0.5 M NaCl by addition of 4M NaCl and then incubated with Ni-NTA-Agarose (10 ml resin) for one hour. The resin was then washed in 10 times with 40 ml of Lysis Buffer containing 0.5M NaCl and then placed in a disposable Econo-Pac column (BioRad), where the resin was further washed with 700 ml of high salt buffer and then with 100 ml of low salt buffer, both supplemented with 10 mM imidazole. Elution was performed with 200 mM imidazole in high salt buffer and 2 ml fractions were collected. Fractions containing protein were pooled, diluted to 200 mM NaCl with 25 mM Tris/HCl pH 7.5, and loaded onto a 5 ml Hi-trap Q sepharose column. The flow-through from this step, containing PDK1, was concentrated to 4 ml and then chromatographed on a 16/60 Superdex 200 gel filtration column using an AKTA Explorer system

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(Amersham Biosciences) equilibrated with high salt buffer with the addition of 1mM DTT. PDK1 eluted in a large symmetric peak at the expected size for a monomer. The PDK1 containing peak was again pooled, concentrated and incubated with 300 µg GST-PreScission protease (expression construct kindly provided by John Heath, University of Birmingham, UK) on ice for 4h. In order to eliminate the cleaved His-tag sequences as well as any remaining uncleaved His-PDK1 and the GST-PreScission protease, the mixture was incubated with a mixture of 200 µl glutathione-Sepharose and

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remaining uncleaved His-PDK1 and the GST-PreScission protease, the mixture was incubated with a mixture of 200 μ l glutathione-Sepharose and 200 μ l Ni-NTA agarose resin for 15 minutes and the PDK1 protein that did not bind was collected. The resulting protein consists of PDK1 (51-359) preceded by a Gly-Pro at the N-terminus. The protein at this stage of the purification was apparently homogeneous as revealed by a single band after electrophoresis of 20 μ g of protein on SDS-PAGE and staining with

Coomasie Brilliant Blue R250 (data not shown).

Electrospray mass spectrometry revealed a main peak mass close to the expected size of this fragment of PDK1. The specific activity of PDK1 (51-359) towards the peptide T308tide and its activation in the presence of PIFtide was identical to wild type full length PDK1 [Biondi et al., 2000], and tryptic peptide mass finger printing indicated that PDK1 was quantitatively phosphorylated at Ser241 (data not shown). In BiaCore experiments, the steady state binding of PDK1 (51-359) to the peptide PIFtide was similar to that of the His-tag PDK1 (51-556) protein characterised previously [Balendran et al., 1999a].

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Crystallisation and data collection

The PDK1 (51-359) protein was concentrated to a final concentration of 8.5 mg/ml (as determined by a Bradford assay using bovine serum albumin as a

standard). The sitting drop vapour diffusion method was used for producing crystals. Sitting drops were formed by mixing 1 µl of protein solution with 1 µl of a mother liquor solution (0.1 M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP) with the addition of 0.2 µl EDTA (100mM). Hexagonal crystals (Table I) of PDK1 were grown at 20° C from a mother liquor containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP). Crystals appeared after one day, growing to 0.05 x 0.05 x 0.2 mm over 20 days. Crystals were frozen in a nitrogen gas stream after being soaked in 0.075 M Tris 8.5, 1.5M ammonium sulphate, 25% (v/v) glycerol.

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Expression and purification of wild type and mutant forms of GST-PDK1.

Wild type-PDK1 [Alessi et al., 1997], PDK1[R76A], PDK1[R131A], PDK1[R76A,R131A], PDK1[T148A] and PDK1[Q150A] in the pEBG2T vector were used to express the wild type and indicated mutants of PDK1 fused through their N-terminus to glutathione S-transferase (GST). The GST fusion proteins were expressed in human embryonic kidney 293 cells. For the expression of each construct, twenty 10 cm diameter dishes of 293 cells were cultured and each dish transfected with 10 μg of the pEBG-2T construct, using a modified calcium phosphate method. 36 h post-transfection, the cells were lysed in 0.6 ml of ice-cold Buffer A, the lysates pooled, centrifuged at 4 °C for 10 min at 13000 g and the GST-fusion proteins were purified by affinity chromatography on glutathione-Sepharose and eluted in Buffer B supplemented with 20 mM glutathione as described previously [Alessi et al., 1997]. Typically between 1 and 2mg of each GST-fusion protein was obtained and each protein was more than 75 judged by SDS polyacrylamide gel electrophoresis (data not shown).

PDK1 catalytic activity measurements

The ability of wild type and mutant PDK1 to phosphorylate the synthetic peptide T308tide (KTFCGTPEYLAPEVRR ([Biondi et al., 2000]) was carried out in 30 µl assays containing 100 ng of wild type or mutant PDK1, 50 mM Tris/HCl pH 7.5, 0.1% β -mercaptoethanol, 10 mM MgCl₂, 100 μ M [32y P]ATP (200 cpm/pmol), 0.5 µM microcystin-LR, 1 mM T308tide in the presence or absence of the indicated concentrations of the S6K-pHM S6K-HM.peptide (SESANQVFLGFT(P)YVAPSV) peptide (SESANQVFLGFTYVAPSV). After incubation for 10 min at 30 °C, 25 µl of the resultant mixture was spotted into P81 phosphocellulose paper (2 x 2 cm) and the papers washed and analysed as described previously for assays of MAP kinase. Control assays were carried out in parallel in which either PDK1, or peptide substrate were omitted; these values were always less than 5% of the activity measured in the presence of these reagents. One Unit of PDK1 activity was defined as that amount required to catalyse the phosphorylation of 1 nmol of the T308tide in 1 min.

Biacore analysis

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Binding was analysed in a BiaCore 3000 system (BiaCore AB, Stevenage, UK). Biotinylated S6K-pHM (Biotin-C₁₂- SESANQVFLGFT(P)YVAPSV) or the non-phosphorylated form of this peptide S6K-HM was bound to an streptavidin- coated Sensor chip (SA) (12 response units, RU). 30 μl of wild type or the indicated mutant GST-PDK1 were injected at a flow rate of 30μl/min, in buffer HBS-P (10 mM HEPES pH 7.4, 0.15M NaCl, 0.005% (by vol) polysorbate-20) supplemented with 1 mM DTT. Specific interactions between S6K-pHM and PDK1 proteins were obtained between the concentration range of 2-2150 nM PDK1. Steady state binding was

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determined at each concentration. Dissociation of PDK1 from the phosphopeptide was monitored over a 1min period. Regeneration of the sensor chip surface was performed with 10µl injections of 0.05% SDS. As previously found for PDK1 binding to PIFtide [Biondi et al., 2000], the interaction data obtained using BiaCore did not fit to simple 1:1 interaction model. Apparent Kd values were estimated from the concentration of PDK1 which gives 50% of maximal response, which was obtained empirically using GST-PDK1[T148A] (RUmax=435). For all PDK1 construct tested, the off rates for S6Kp-HM were high in comparison to those of PIFtide binding with the time taken for 50% dissociation to occur for S6K-pHM is 30s compared to 1000s for PIFtide. This could account for the overall approximately 100-fold lower affinity of wild type PDK1 for S6K-pHM in comparison to PIFtide.

15 Data collection, structure solution, and refinement

Data on PDK1 crystals were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH1, using an ADSC Q4 CCD detector. The temperature of the crystals was maintained at 100K using a nitrogen cryostream. Data were processed using the HKL package [Otwinowski and Minor, 1997], statistics are shown in Table I.

The structure of PDK1 was solved by molecular replacement with AMoRe [Navaza, 1994] using the structure of PKA in complex with an inhibitory peptide as a search model (PDB entry 1YDB), against 8-4 Ådata. A single, well separated solution was found with an R-factor of 0.479 (correlation coefficient = 0.428). The structure was automatically built using warpNtrace [Perrakis et al., 1999], which found 262 of a possible 309 residues, giving an initial protein model with R=0.293 (Rfree=0.318) after

ated annealing in CNS [

simulated annealing in CNS [Brunger et al., 1998]. Iterative protein building in O [Jones et al., 1991] together with refinement in CNS, which included incorporation of a model for ATP, the phosphoserine in the activation loop, solvent molecules and a key sulphate molecule, resulted in a final model with R=0.195 (Rfree=0.222). No electron density was observed for residues 51-70 (the N-terminus of the construct) and 233-236 (the tip of the activation loop). All figures were made with PyMOL (http://www.pymol.org).

10 Table I

Details of data collection & structure refinement for the PDK1 kinase domain. Values between brackets are for the highest resolution shell. All measured data were included in structure refinement.

15 : Wave length ()

0.933

Space group

P3₂21

Unit cell ()

a=123.01, b=123.01, c=47.62

Resolution ()

25-2.0 (2.07-1.0)

Observed reflections

77315

Unique reflections

27643

Redundancy

2.8 (2.5)

Completeness(%)

98.0 (93.5)

Rmerge

20

0.091 (0.454)

I/ sigma I

7.3 (2.0)

25 R_{free} reflections

579

R_{crvst}

0.195

 R_{free}

0.222

Number of groups

°°Protein residues

71-359

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		62
	°°Water	200
	ATP	1
	SO ₄	5
	Glycerol	` 8
5	Wilson B (2)	22.4
	Protein	25.6
	< B > Water	35.7
	< B > ATP	38.8
	RMSD from ideal geometry	
0	Bond lengths ()	0.005
	Bond angles (°)	1.34
	Main chain B (2)	1.5.

References

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Example 2: Co-ordinates for PDK1 fragment with all alternate side chains.

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REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free_r= 0.2220
                    r= 0.1954 free_r= 0.2224
    REMARK final
    REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0
    REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
    REMARK rweight= 0.0900 (with wa= 1.29263)
10
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1 : /dd1/david/projects/PDK1_new/CNS/prot.par
    REMARK parameter file 2 : /ddl/david/projects/PDK1_new/CNS/atp.par
15
    REMARK parameter file 3 : CNS_TOPPAR:water_rep.param

REMARK parameter file 4 : CNS_TOPPAR:ion.param

REMARK parameter file 5 : /ddl/david/projects/PDK1_new/CNS/glycerol.par
    REMARK molecular structure file: ../generate/alternate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
20
    REMARK reflection file= ../../1/hkl/cns.hkl
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.0
    REMARK initial B-factor correction applied to fobs :
    REMARK B11= -2.766 B22= -2.766 B33=
REMARK B12= -0.375 B13= 0.000 B23=
                                               5.532
25
                                                0.000
     REMARK B-factor correction applied to coordinate array B:
     REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
    REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
                                                                     28210 ( 100.0
     REMARK theoretical total number of refl. in resol. range:
                                                                               2.0
    REMARK number of unobserved reflections (no entry or |F|=0):
                                                                       568 (
     ୫ )
                                                                               0.0
     REMARK number of reflections rejected:
35
     ቄ )
                                                                     27642 ( 98.0
     REMARK total number of reflections used:
                                                                     27063 (
                                                                              95.9
     REMARK number of reflections in working set:
     용 )
                                                                       579 (
                                                                               2.1
     REMARK number of reflections in test set:
                                 47.624 90.00 90.00 120.00 P 32 2 1
     CRYST1 123.013 123.013
     REMARK FILENAME="bindividual.pdb"
     REMARK DATE:16-Apr-2002 18:31:12 ' created by user: david
45
     REMARK VERSION:1.0
               1 CB PRO A 71
                                   58.912 -7.251
                                                    8.216 1.00 67.78 A
     MOTA
                                                    9.534 1.00 69.16 A
               2 CG PRO A 71
                                   59.621 -6.941
     MOTA
                                           -6.506
                                                    5.894 1.00 67.06
               3 C
                      PRO A
                             71
                                   59.493
     ATOM
                                                            1.00 66.66
                                   59.196
                                           -5.318
                                                    5.766
               4 0
                      PRO A
                             71
50
     MOTA
                                                            1.00 67.86 A
               5 N
                                   60.984
                                           -6.073
                                                     7.833
                       PRO A
                              71
     MOTA
                                                    9.207
                                                            1.00 68.24 A
                                           -5.762
               6 CD
                      PRO A
                              71
                                   60.554
     MOTA
                                                    7.217
                                           -7.035
                                                            1.00 67.75 A
                                   60.040
               7
                  CA
                      PRO A
                              71
     MOTA
                                                    4.890 1.00 66.32 A
               8 N
                       PRO A 72
                                   59.356 -7.385
     ATOM
                                                    4.898 1.00 67.17 A
                                   59.712 -8.816
               9
                  CD
                      PRO A 72
55
     MOTA
                                                    3.578 1.00 65.61 A
              10 CA PRO A 72
                                   58.840 -6.986
     MOTA
                                                    2.858 1.00 66.47
              11 CB
                      PRO A 72
                                   58.672 -8.321
     MOTA
                                                    3.419 1.00 67.57 A
              12 CG PRO A 72
                                   59.796 -9.133
     MOTA
```

	ATOM	13	С	PRO A	72	57.527	-6.208	3.673	1.00		A
	MOTA	14	0	PRO A	72	56.710	-6.451	4.561	1.00	64.11	A
	MOTA	15	N	ALA A	73	57.341	-5.268	2.753	1.00	61.57	A
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708	1.00	58.74	A
5	ATOM	17	CB	ALA A	73	56.438	-3.030	3.165	1.00	58.05	Α
	MOTA	18	С	ALA A	73	55.626	-4.448	1.271	1.00	56.78	Α
	ATOM	19	0	ALA A	73	56.347	-4.834	0.349	1.00	56.95	Α
	ATOM	20	N	PRO A	74	54.372	-4.024	1.057	1.00	54.15	A
	ATOM	21	CD	PRO A	74	53.335	-3.610	2.018	1.00	53.31	Α
10	ATOM	22	CA	PRO A	74	53.856	-4.003	-0.314	1.00	52.54	Α
	ATOM	23	СВ	PRO A	74	52.474	-3.375	-0.148	1.00	52.86	Α
	ATOM	24	CG	PRO A	74	52.067	-3.824	1.226		52.88	Α
	ATOM	25	C	PRO A	74	54.772	-3.167	-1.204	1.00	50.08	Α
	ATOM	26	o	PRO A	74	55.559	-2.361	-0.708		49.96	A
15		27	N	ALA A	75	54.680	-3.366	-2.514		47.58	A
15	ATOM		CA	ALA A	75	55.503	-2.602	-3.446		44.69	A
	ATOM	28		ALA A	75	55.312	-3.121	-4.870		46.14	A
	ATOM	29	СВ				-1.134	-3.371		41.55	Α
	ATOM	30	C	ALA A	75	55.100		-3.086		41.01	A
	MOTA	31	0	ALA A	75	53.947	-0.813			38.31	A
20	MOTA	32	N	LYS A	76	56.053	-0.245	-3.619			A
	MOTA	33	CA	LYS A	76	55.781	1,184	-3.588		35.72	
	MOTA	34	CB	LYS A	76	57.053	1.957	-3.930		37.70	A
	MOTA	35	CG	LYS A	76	57.123	3.356	-3.350		40.99	A
	ATOM	36	CD	LYS A	76	57.262	3.316	-1.836		40.04	A
25	MOTA	37	CE	LYS A	76	57.511	4.705	-1.277		42.08	A
	MOTA	38	NZ	LYS A.	76	57.681	4.695	0.202		42.99	A
	MOTA	. 39	С	LYS A	76	54.708	1.467	-4.638		32.65	A
	ATOM	40	0	LYS A	76	54.814	1.005	-5.770		31.41	A
•	MOTA	41	N	LYS A	77	53.668	2.207	-4.270		28.59	A
30	MOTA	42	CA	LYS A	77	52.619	2.517	-5.232	1.00		A
	ATOM	43	CB	LYS A	77	51.316	2.865	-4.509		26.22	A
	MOTA	44	CG	LYS A	77	50.796	1.731	-3.631	1.00	27.15	Α
	ATOM	45	CD	LYS A	77	49.487	2.089	-2.967		26.80	Α
	ATOM	46	CE	LYS A	77	49.136	1.091	-1.870		27.31	A
35	ATOM	47	NZ	LYS A	77	48.998	-0.296	-2.380	1.00	27.17	Α
	ATOM	48	C	LYS A	77	53.053	3.668	-6.137	1.00	24.67	Α
	ATOM	49	0	LYS A	77	54.010	4.377	-5.829		21.60	A
	ATOM	50	N	ARG A	78	52.351	3.838	-7.254		23.66	Α
	ATOM	51	CA	ARG A	78	52.662	4.897	-8.211		26.14	Α
40	ATOM	52	CB	ARG A	78	53.574	4.344	-9.318	1.00	28.57	Α
	ATOM	53	CG	ARG A	78	53.017	3.139	-10.050	1.00	34.7B	Α'
	ATOM	54	CD	ARG A	78	54.092	2.465	-10.896	1.00	40.96	A
	MOTA	55	NE	ARG A	78	53.560	1.364	-11.700	1.00	48.93	Α
	ATOM	56	CZ	ARG A	78	52.985	0.270	-11.203	1.00	52.58	Α
45	ATOM	57	NH1	ARG A	78	52.860	0.113	-9.889	1.00	54.60	Α
	ATOM	58	NH2	ARG A	78	52.530	-0.672	-12.022	1.00	54.09	Α
	ATOM	59	С	ARG A	78	51.382	5.488	-8.803	1.00	23.76	Α
	ATOM	60	O	ARG A	78	50.311	4.888	-8.706	1.00	24.25	Α
	ATOM	61	N	PRO A	79	51.475	6.676	-9.428		21.76	Α
50	ATOM	62	CD	PRO A	79	52.691	7.475	-9.668	1.00	20.82	Α
50	ATOM	63	CA	PRO A	79	50.301		-10.021		21.96	A
	ATOM	64	CB	PRO A	79	50.910		-10.816	1.00	22.27	
	ATOM	65	CG	PRO A	79	52.124		-10.014		22.12	
	ATOM	66	C	PRO A	79	49.446		-10.903		22.86	
55	ATOM	67	o	PRO A	79	48.213		-10.842	-	20.52	
"	ATOM	68	N	GLU A	80	50.103		-11.714		21.87	
		69	CA	GLU A	80	49.403		-12.628		22.99	
	ATOM	70	CB	GLU A		50.393	3.994 -		0.50 2		AC1
	ATOM	71	CG	GLU		51.230	2.907 -		0.50 2		AC1
	MOTA	, 1	ÇĞ	010	80	J1.230			2		

			<i>a</i> n	OT 11		F0 1F2	2.224	12 0	12 0 50	31.99 AC1	
	MOTA	72		GLU		52.157 53.072	2.224			34.34 AC1	
	MOTA	73	OE1			51.969	1.015			32.83 AC1	
	ATOM	74		GLU A	80	48.556		1 -11		00 22.09 A	
5	ATOM	75 76	C O	GLU A	80	47.692		3 -12		00 22.37 A	
)	ATOM		N	ASP A	81	48.804		3 -10		00 19.97 A	
	ATOM	77	CA	ASP A	81	48.026	2.42			00 19.93 A	
	ATOM	78 79	CB	ASP A	81	48.736	2.02			00 21.19 A	
	ATOM	80	CG	ASP A	81	50.089	1.38			00 22.46 A	
10	ATOM	81		ASP A	81	50.195	0.55			00 24.22 A	
10	MOTA	82		ASP A	81	51.0		.685	-8.058	1.00 23.33	A
	ATOM	83	C	ASP A	81	46.6		.975	-9.518	1.00 20.85	A
	ATOM	84	0	ASP A	81	45.		.246	-9.015	1.00 19.96	A
•	MOTA MOTA	85	И	PHE A	82	46.4		.258	-9.804	1.00 18.91	A
15	ATOM	86	CA	PHE A	82	45.2		.934	-9.465	1.00 19.30	A
1,7	ATOM	87	CB	PHE A	82	45.4		.027	-8.427	1.00 18.43	A
	ATOM	88	CG	PHE A	82	46.		.531	-7.175	1.00 18.01	A
	ATOM	89		PHE A	82	45.		.136	-6.084	1.00 17.19	A
	ATOM	90		PHE A	82	47.		.460	-7.086	1.00 18.99	A
20	ATOM	91		PHE A	82			.676	-4.918	1.00 17.12	Α
20	ATOM	92	CE2		82			.000	-5.925	1.00 19.64	Α
	ATOM	93	CZ	PHE A	82			.607	-4.838	1.00 18.00	A
	ATOM	94	C	PHE A	82				-10.621	1.00 20.81	A
	ATOM	95	Ö	PHE A	82				-11.649	1.00 20.34	Α
25	ATOM	96	N	LYS A	83				-10.411	1.00 19.80	Α
23	ATOM	97	CA	LYS A	83			.478	-11.353	1.00 21.65	Α
	ATOM	98	CB	LYS A	83				-11.687	1.00 22.02	Α
	ATOM	99	CG	LYS A	83				-12.550	1.00 28.93	Α
	ATOM	100	CD	LYS A	83				-12.981	1.00 34.20	A
30	ATOM	101	CE	LYS A	83				-13.824	1.00 38.10	A
50	ATOM	102	NZ	LYS A	83				-13.043	1.00 43.33	A
	ATOM	103	C	LYS A	83			.702	-10.541	1.00 20.74	A
	ATOM	104	ŏ	LYS A	83			.606	-9.635	1.00 20.98	A
	MOTA	105	N	PHE A	84			.848	-10.835	1.00 19.99	A
35	ATOM	106	CA	PHE A	84			.049	-10.083	1.00 18.63	Α
55	ATOM	107	CB	PHE A	84				-10.258	1.00 18.95	Α
	MOTA	108	CG	PHE A	84			.741	-9.587	1.00 17.68	A
	ATOM	109		PHE A	84		498 9	9.926	-10.224	1.00 18.16	A
	ATOM	110		PHE A	84		843 13	1.183	-8.299	1.00 19.66	Α
40	ATOM	111		PHE A	84	_		9.556	-9.589	1.00 18.09	A
-10	ATOM	112		PHE A	84		021 10	.816	-7.653	1.00 18.89	A
	ATOM	113	CZ	PHE A	84		936 10	.002	-8.301	1.00 17.33	Α
	ATOM	114	C	PHE A	84	40.	834 10	0.617	-10.460	1.00 19.69	A
	ATOM	115	0	PHE A	84	40.	391 10	.489	-11.601	1.00 20.72	Α
45	ATOM	116	N	GLY A	85	40.	178 13	1.233	-9.484	1.00 16.80	A
	ATOM	117	CA	GLY A	85	38.	872 13	1.810	-9.716	1.00 17.73	A
	ATOM	118	С	GLY A	85	38.	819 13	3.280	-9.346	1.00 18.75	, A
•	ATOM	119	0	GLY A	85	39.	740 14	1.043	-9.650	1.00 18.45	A
	MOTA	120	N	LYS A	86	37.	753 13	3.673	-8.659	1.00 16.00	A
50	MOTA	121	CA	LYS A	86	37.	571 1	5.064	-8.278	1.00 18.26	A
50	ATOM	122	CB	LYS A				5.302	-7.812	1.00 19.00	A
	ATOM	123	CG	LYS A				4.660		1.00 21.55	A
	MOTA	124	CD	LYS A		5 34.	368 1	4.981	-6.066		A
	ATOM	125	CE	LYS A				4.239		1.00 31.92	A
55	ATOM	126	NZ	LYS A		32.		4.457		1.00 35.36	A
-	ATOM	127	С	LYS A	8	5 38.		5.571			A
	ATOM	128	0	LYS A		5 39.		4.807			A
	MOTA	129	N	ILE A				6.881			A
	MOTA	130	CA	ILE A	. 8'	7 39	.577 1	7.554	-6.256	1.00 18.26	A

	ATOM	131	CB	ILE	Α	87	39	.994	18.952	-6.772		19.60	A
	MOTA	132	CG2	ILE	A	87	40	.593	19.786	-5.628		18.73	A
	ATOM	133	CG1	ILE	Α	87	40	.968	18.786	-7.945		21.16	A
	ATOM	134	CD1	ILE	Α	87		.412	20.087	-8.588		25.26	A
5	ATOM	135	С	ILE	A	87		.731	17.709	-4.997		19.67	A
	MOTA	136	0	ILE	Α	87	37	.628	18.249	-5.052		20.41	A
	MOTA	137	N	LEU	Α	-88	39	.240	17.229	-3.867		19.15	A
	ATOM	138	CA	LEU	Α	88	38	.508	17.324	-2.611		20.68	A
	ATOM	139	CB	LEU	Α	88	38	8.870	16.151	-1.700		19.97	A
10	ATOM	140	CG	LEU	Α	88	38	3.529	14.759	-2.237		19.24	A
	ATOM	141	CD1	LEU	A	88	3 9	0.090	13.692	-1.311		21.41	A
	ATOM	142	CD2	LEU	Α	88	37	1.029	14.622	-2.359		18.84	A
	ATOM	143	C	LEU	Α	88	3 8	3.815	18.632	-1.901		23.11	A
	ATOM	144	0	LEU	Α	88	37	7.999	19.146	-1.139		25.10	A
15	ATOM	145	N	GLY	A	89	39	9.997	19.174	-2.149		24.09	A
	ATOM	146	CA	GLY	Α	89	40	367	20.418	-1.507		24.27	A
	ATOM	147	С	GLY	Α	89	4:	1.658	20.954	-2.078		25.47	A
	ATOM	148	0	GLY	Α	89	42	2.445	20.202	-2.666		22.19	A
	ATOM	149	N	GLU	Α	90	4	1.870	22.254	-1.906		26.22	A
20	MOTA	150	CA	GLU	A	90	43	3.064	22.924	-2.404		29.96	A
	MOTA	151	CB	GLU	Α	90	42	2.698	23.814	-3.596		30.75	A
	ATOM	152	CG	GLU	Α	90	42	2.267	23.038	-4.831		34.32	A
	ATOM	153	CD	GLU	Α	90	4:	1.711	23.930	-5.927		38.27	A
	ATOM	154	OE1	GLU	Α	90	4	0.590	24.456	-5.764		40.57	A
25	ATOM	155	OE2	GLU	Α	90	4:	2.398	24.110	-6.952		40.90	A
	MOTA	156	C	GLU	Α	90	4	3.711	23.768	-1.313		30.68	A
	MOTA	157	0	GLU	Α	90	4	3.049	24.574	-0.668		32.83	A
	ATOM	158	N	GLY	Α	91	4	5.006	23.566	-1.104		29.66	A
	MOTA	159	CA	GLY	Α	91	4	5.724	24.332	-0.104		29.40	A
30	ATOM	160	C	GLY	Α	91	4	6.795	25.151	-0.798		29.98	A
	ATOM	161	Ö	GLY	Α	91	4	6.894	25.130	-2.028		28.16	A
	ATOM	162	N	SER	A	92	4	7.605	25.870	-0.029		28.30	A
	MOTA	163	CA	SER	Α	92	4	8.653	26.681	-0.633		30.50	A
	ATOM	164	CB	SER	Α	92	4	9.165	27.717	0.370		32.43	A
35	ATOM	165	OG	SER	Α	92	4	9.520	27.099	1.593		40.94	A
	ATOM	166	C	SER	Α	92	4	9.815	25.843	-1.164		29.77	A
	MOTA	167	0	SER	A	92	5	0.456	26.221	-2.143		30.46	A
	MOTA	168	N	PHE	A	93	5	0.087	24.703	-0.536		27.65	A
	ATOM	169	CA	PHE	A	93	5	1.185	23.855	-0.995		26.34	A
40	MOTA	170	CB	PHE	A	93	5	2.281	23.785	0.068		27.95	A
	MOTA	171	CG	PHE	A	93	5	2.861	25.117	0.406		31.06	A
	MOTA	172	CD1	LPHE	Α	93	5	2.283	25.909	1.392		29.96	A
	ATOM	173	CD2	PHE	A	93	5	3.949	25.613	-0.308		31.38	A
	MOTA	174	CEI	L PHE	E A	93	5	2.779	27.181	1.665		32.69	A
45	ATOM	175	CE	2 PHE	A 2	93	5	4.452	26.883	-0.044		32.63	A
	ATOM	176	CZ	PHI	E A	93	5	3.864	27.670	0.945		31.81	A
	ATOM	177	C	PHE	E A	93	5	0.759	22.445	-1.365		25.39	A
	ATOM	.178	0	PHI	ΞΑ	93	5	1.601	21.559	-1.522		0 24.59	A
	ATOM	179	N	SEI			4	9.457	22.235	-1.519		0 23.63	A
50	ATOM	180	CA	SEI	R A	94	4	8.965	20.912	-1.860		0 21.43	A
50	ATOM	181	СВ	SEI			4	19.017	20.013	-0.628		0 21.42	A
	ATOM	182	OG		R A		4	8.091	20.475	0.340		0 21.19	A
	ATOM	183		SE			4	17.539	20.925	-2.378		0 19.82	A
	ATOM	184	ō	SE			4	16.795	21.882	-2.173		0 18.76	A
55	ATOM	185	N		R A		4	17.174	19.832	-3.038		0 19.38	A
,,	ATOM	186			R A		. 4	15.840	19.637	-3.580		0 17.98	A
	ATOM	187			R A		4	45.818	19.818	-5.110		0 19.25	A
	MOTA	188		1 TH				46.196	21.162	-5.434		0 22.04	A
	ATOM	189		2 TH			4	44.421	19.549	-5.661	1.0	0 17.61	A
					-	_							

	MOTA	190	С	THR	Α	95		45.455	18.201	-3.243	1.00 18.61	. А
	ATOM	191	0	THR	Α	95		46.212	17.264	-3.524	1.00 17.10) A
	ATOM	192	N	VAL	Α	96		44.295	18.024	-2.623	1.00 16.53	a A
	ATOM	193	CA	VAL	A	96		43.845	16.685	-2.266	1.00 16.05	
5	MOTA	194	CB	VAL	Α	96		43.170	16.672	-0.886	1.00 16.32	
	ATOM	195	CG1	VAL	Α	96		42.741	15.249	-0.532	1.00 18.02	_
	MOTA	196	CG2	VAL	Α	96		44.145	17.206	0.168	1.00 16.69	_
	ATOM	197	C	VAL	Α	96		42.875	16.207	-3.335	1.00 16.42	
	ATOM	198	0	VAL	A	96		41.906	16.892	-3.665	1.00 16.47	
10	ATOM	199	N	VAL	Α	97		43.157	15.033	-3.888	1.00 16.80	
	ATOM	200	CA	VAL	A	97		42.338	14.471	-4.949	1.00 16.72	
	MOTA	201	CB	VAL	Α	97		43.153	14.354	-6.255	1.00 18.43	
	ATOM	202	CG1	VAL	Α	97		42.249	13.927	-7.404	1.00 19.69	
	ATOM	203	CG2	VAL	Α	97		43.831	15.685	-6.569	1.00 17.84	
15	ATOM	204	С	VAL	Α	97		41.812	13.091	-4.583	1.00 16.7	_
	ATOM	205	0	VAL	Α	97		42.532	12.270	-4.014	1.00 17.1	
	ATOM	206	N	LEU	Α	98		40.545	12.845	-4.895	1.00 16.63	_
	MOTA	207	CA	LEU	Α	98		39.947	11.548	-4.624	1.00 17.0	
	MOTA	208	CB	LEU	Α	98		38.424	11.633	-4.743	1.00 16.8	
20	ATOM	209	CG	LEU	Α	98		37.635	10.342	-4.508	1.00 19.4	
	MOTA	210	CD1	LEU	Α	98		37.990	9.762	-3.146	1.00 20.0	
	MOTA	211	CD2	LEU	A	98		36.143	10.627	-4.588	1.00 17.9	
	MOTA	212	C	LEU	Α	98		40.512	10.597	-5.677	1.00 17.3	
	MOTA	213	0	LEU	Α	98		40.527	10.920	-6.863	1.00 18.6	
25	ATOM	214	. N	ALA	A	99		40.995	9.438	-5.246	1.00 17.1	
	MOTA	215	CA	ALA	A	99		41.570	8.466	-6.168	1.00 18.4	
	MOTA	216	CB	ALA	. A	99		43.090	8.524	-6.105	1.00 14.7	
	MOTA	217	C	ALA	A	99		41.102	7.055	-5.848	1.00 21.4	
	MOTA	218	0	ALA	A	99		40.941	6.691	-4.679	1.00 22.5	_
30	MOTA	219	N	ARG	Α	100		40.878	6.261	-6.888	1.00 19.7	_
	MOTA	220	CA			100		40.459	4.884	-6.693	1.00 20.8	
	MOTA	221	CB	ARG	Α	100		39.202	4.585	-7.518	1.00 24.2	_
	MOTA	222	CG	ARG	A	100		38.608	3.205	-7.256	1.00 31.7	
	MOTA	223	CD			100		37.326	2.979	-8.048	1.00 36.2	
35	MOTA	224	NE			100		36.213	3.818	-7.594	1.00 41.4	_
	MOTA	225	CZ			100		35.566	3.662	-6.439	1.00 42.0	_
	MOTA	226		ARG				35.912	2.696	-5.598	1.00 40.6	-
	MOTA	227	NH2	ARG			•	34.559	4.468	-6.128	1.00 43.6	
	MOTA	228	С			100		41.613	3.985	-7.129	1.00 18.6	_
40	MOTA	229	0			100		42.078	4.065	-8.271	1.00 19.4 1.00 16.4	_
	ATOM	230	N			101		42.102	3.157	-6.212	1.00 16.4	•
	MOTA	231	CA			101		43.196	2.246	-6.533	1.00 16.7	_
	MOTA	232	CB			101		43.774	1.637	-5.248	1.00 16.5	-
	ATOM	233	CG			101		44.917	0.657	-5.488	1.00 18.2	_
45	MOTA	234	CD			101		45.501	0.115	-4.200	1.00 18.2	
	MOTA	235				101		44.733	-0.081	-3.239	1.00 17.1	
	MOTA	236`				101		46.725	-0.132	-4.150	1.00 17.5	
	ATOM	237	С			. 101		42.625	1.152	-7.442	1.00 17.5	
	ATOM	238	0			101		41.681	0.462	-7.069 -8.632	1.00 10.0	
50	MOTA	239	N			102		43.198	1.002 0.025	-9.607	1.00 20.7	
	ATOM	240	CA			102		42.718		-10.878	1.00 23.4	
	MOTA	241	CB			102		43.569		-11.642	1.00 25.3	
	MOTA	242	CG			102		43.531 44.577		-12.748	1.00 23.8	_
	MOTA	243				102		44.5//		-12.748	1.00 26.7	
55	ATOM	244				102		42.140		-9.125	1.00 21.0	
	MOTA	245	С			102		41.668		-9.305	1.00 21.0	
	. ATOM	246	0			102		43.753		-8.507	1.00 19.3	
	MOTA	247	N			103		43.753		-8.035	1.00 20.	
	MOTA	248	CA	AL	A A	103		4 5.050	3.243	0.000		

	ATOM	249	CB	ALA	Α	103	45.28	4	-3.571	-7.671	1.00	19.23	A
	ATOM	250	Ĉ.	ALA	Α	103	42.91	.9	-3.629	-6.872	1.00	19.92	A
	ATOM	251	0	ALA	Α	103	42.70	3	-4.815	-6.628		20.38	A
	ATOM	252	N ,	THR	Α	104	42.36	51	-2.643	-6.175	1.00	18.12	A
5	ATOM	253	CA	THR	Α	104	41.51		-2.927	-5.018		17.15	A
,	ATOM	254	СВ	THR			42.21	.2	-2.484	-3.717		19.54	Α
	ATOM	255		THR			42.45	66	-1.070	-3.773	1.00	19.26	Α
	ATOM	256	CG2				43.53		-3.219	-3.529	1.00	17.02	A
	ATOM	257	C	THR			40.15		-2.247	-5.026	1.00	19.44	A
10	MOTA	258	ō	THR			39.25		-2.648	-4.285	1.00	18.70	A
10		259	Ŋ	SER			40.03		-1.207	-5.847	1.00	19.65	A
	ATOM		CA	SER			38.81		-0.400	-5.967	1.00	19.37	A
	MOTA	260	CB	SER	7.	105	37.59		-1.304	-6.173	0.50	21.81	AC1
	ATOM	261	OG	SER		105	36.43		-0.539	-6.412	0.50	23.01	AC1
1.5	ATOM	262		SER	7		38.64		0.447	-4.701		18.99	A
15	ATOM	263	C			105	37.60		1.070	-4.488		18.66	A
	MOTA	264	0	ARG			39.67		0.468	-3.861		16.84	A
	MOTA	265	N				39.65		1.267	-2.634		16.21	Α.
	MOTA	266	CA	ARG			40.82		0.886	-1.723		16.41	A
••	MOTA	267	CB	ARG			40.6		-0.367	-0.906		15.49	A
20	MOTA	268	CG	ARG					-0.755	-0.170		17.43	A
	ATOM	269	CD	ARG			41.8		-1.792	0.824		20.47	A
	MOTA	270	NE			106	41.6			1.371		20.24	A
	MOTA	271	CZ			106	42.5		-2.568	1.017		17.80	A
	ATOM	272		ARG			43.83		-2.433	2.285		20.14	A
25	MOTA	273		ARG			42.1		-3.468	-2.981		17.37	A
	MOTA	274	C	•		106	39.7		2.746			17.75	A
	MOTA	275	0			106	40.5		3.103	-3.902		16.06	A
	MOTA	276	Ŋ			107	39.0		3.599	-2.240	-	20.80	A
	MOTA	277	CA			107	39.1		5.039	-2.461		22.93	A
30	MOTA	278	CB			107	37.7		5.694	-2.337		30.87	A
	ATOM	279	CG			107	36.7		5.171	-3.269		32.40	A
	MOTA	280	CD			107	35.4		5.975	-3.148		33.74	A
	ATOM	281		r Gra			35.2		6.939	-3.923		36.00	A
	MOTA	282		2 GLU			34.6		5.654	-2.263		18.93	A
35	MOTA	283	C			107	40.0		5.678	-1.410		19.21	A
	MOTA	284	0			107	39.8		5.427	-0.220		16.70	A
	MOTA	285	N			108	40.9		6.507	-1.852		15.86	A
	MOTA	286	CA			108	41.8		7.209	-0.942		15.30	A
	ATOM	287	CB			108	43.3		6.728	-1.104		16.33	A
40	MOTA	288	CG			108	43.5		5.328	-0.612		16.36	A
	MOTA	289		1 TYR	-		43.7		5.066	0.746		18.48	A
	ATOM	290		1 TYR			44.0		3.769			13.25	A
	MOTA	291		2 TYR			43.7		4.268	-1.511		17.28	A
	ATOM	292		2 TYR			43.9		2.981	-1.075		19.17	A
45	MOTA	293	CZ			108	44.1		2.736	0.276		19.38	A
	MOTA	294	OH			108	44.4		1.461	0.688		16.80	A
	MOTA	295	С			108	41.8		8.687	-1.292		15.22	A
	MOTA	296	0			108	41.5		9.058	-2.431		14.61	A
	MOTA	297	N		•	109	42.1		9.528	-0.306		14.30	A
50	MOTA	298	CA			109	42.2		10.957	-0.539			A
	MOTA	299	CB			. 109	41.6		11.726			14.78 16.79	A
	ATOM	300	С			109	43.7		11.136				A
	MOTA	301				109	44.4		10.983			16.52	A
	MOTA	302	N			110	44.1		11.410	-		0 14.80 0 15.80	A
55	MOTA	303				110	45.6		11.574			0 16.85	A
	MOTA	304				110	46.0		10.863			0 16.80	A
	MOTA	305		2 ILE			47.5		11.098			0 15.86	A
	MOTA	306		1 ILE			45.7		9.358			0 17.76	A
	ATOM	307	CD	1 ILE	3 A	110	46.3	308	8.513	-4.437	1.0	0 10.07	A

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	ATOM	308	С	ILE	Α :	110		46.004	13.045	-2.129	1.00 17.78	A
	ATOM	309	0	ILE 2	A :	110		45.534	13.813	-2.976	1.00 16.24	A
	ATOM	310	N	LYS 3	Α :	111		46.846	13.435	-1.177	1.00 16.15	A
	ATOM	311	CA	LYS .	A :	111		47.326	14.808	-1.100	1.00 17.20	A
5	ATOM	312	CB	LYS .				47.700	15.176	0.344	1.00 17.41	A
_	ATOM	313	CG.	LYS .				48.350	16.547	0.464	1.00 20.71	A
	ATOM	314	CD	LYS	A :	111		48.585	16.971	1.910	1.00 24.25	Α
	ATOM	315	CE	LYS				47.288	17.381	2.598	1.00 29.46	A
	ATOM	316	NZ	LYS				47.516	17.866	4.000	1.00 30.50	A
10	ATOM	317	C	LYS				48.551	14.890	-1.994	1.00 16.41	A
	ATOM	318	ō	LYS				49.509	14.137	-1.813	1.00 18.20	A
	ATOM	319	N	ILE				48.509	15.798	-2.963	1.00 15.87	A
	ATOM	320	CA	ILE				49.606	15.967	-3.907	1.00 17.28	A
	ATOM	321	CB	ILE				49.079	15.911	-5.358	1.00 16.43	A
15	ATOM	322		ILE				50.235	15.998	-6.341	1.00 15.12	A
13	ATOM	323		ILE				48.293	14.609	-5.565	1.00 16.82	A
	ATOM	324		ILE				47.580	14.511	-6.904	1.00 18.47	A
	ATOM	325	C	ILE				50.307	17.301	-3.663	1.00 19.03	A
	ATOM	326	ō	ILE				49.669	18.350	-3.635	1.00 19.15	A
20	ATOM	327	N	LEU				51.622	17.245	-3.472	1.00 20.22	A
20	ATOM	328	CA	LEU				52.416	18.442	-3.214	1.00 22.36	A
	MOTA	329	CB	LEU				52.995	18.397	-1.794	1.00 22.13	A
	ATOM	330	CG	LEU				52.042	18.063	-0.646	1.00 22.46	A
	MOTA	331		LEU				51.866	16.557	-0.553	1.00 23.81	A
25	ATOM	332		LEU				52.603	18.595	0.660	1.00 23.68	. A
23	ATOM	333	C	LEU				53.560	18.547	-4.215	1.00 23.37	Α
	ATOM	334	ō	LEU			•	54.300	17.586	-4.424	1.00 23.11	A
	ATOM	335	N	GLU				53.706	19.714	-4.834	1.00 23.88	A
	ATOM	336	CA	GLU	Α	114		54.771	19.920	-5.806	1.00 26.00	A
30	ATOM	337	CB	GLU	Α	114		54.435	21.111	-6.706	1.00 27.74	A
-	ATOM	338	CG	GLU	Α	114		55.533	21.452	-7.696	1.00 35.07	A
	MOTA	339	CD	GLU	A	114		55.220	22.696	-8.497	1.00 39.24	A
	MOTA	340	OE1	GLU	Α	114		54.808	23.703	-7.885	1.00 41.45	A
	ATOM	341	OE2	GLU	Α	114		55.395	22.670	-9.736	1.00 44.05	A
35	ATOM	342	С	GLU	Α	114		56.087	20.163	-5.067	1.00 24.37	A
	ATOM	343	0	GLU	Α	114		56.186	21.071	-4.238	1.00 24.43	A
	ATOM	344	N	ĻYS	A	115		57.096	19.350	-5.360	1.00 24.10	A
	ATOM	345	CA	LYS	A	115		58.376	19.493	-4.678	1.00 24.93	A
	MOTA	346	CB	LYS				59.339	18.373	-5.103	1.00 23.72	A
40	ATOM	347	CG	LYS				59.139	17.080	-4.308	1.00 23.09	A A
	MOTA	348	CD	LYS				60.064	15.944	-4.743	1.00 21.92	A
	MOTA	349	CE	LYS				59.691	15.400	-6.117	1.00 22.42 1.00 19.71	A
	MOTA	350	NZ	LYS				60.447	14.150	-6.448	1.00 19.71	A
	ATOM	351	C	LYS				59.031	20.858	-4.868	1.00 26.87	A
45	MOTA	352	0			115		59.492	21.469	-3.903	1.00 28.73	A
	MOTA	353	N			116		59.058	21.348	-6.102	1.00 28.73	A
	MOTA	354	CA		A.	116		59.678	22.638	-6.380	0.50 31.29	AC1
	ATOM	355	CB	ARG		116		59.533	22.980	-7.868 -8.267	0.50 33.19	AC1
	MOTA	356	CG	ARG		116		60.047	24.361 24.710	-7.590	0.50 35.13	AC1
50	ATOM	357	CD	ARG		116		61.368	23.612	-7.618	0.50 36.42	AC1
	ATOM	.358	NE	ARG		116		62.329 63.510	23.648	-7.010	0.50 36.18	AC1
	MOTA	359	CZ	ARG		116		63.871	24.729	-6.332	0.50 36.12	AC1
	MOTA	360		ARG		116 116		64.324	22.602	-7.067	0.50 35.77	AC1
	MOTA	361		ARG		116		59.097		-5.519	1.00 29.70	A
55	MOTA	362	C			116		59.843	24.515	-4.889	1.00 29.16	A
	ATOM	363 364	N O			117		57.773		-5.472	1.00 27.22	A
	MOTA	365	CA			117		57.126			1.00 26.33	A
	MOTA	365 366				117		55.606			1.00 28.41	A
	ATOM	200	CD	1110	-							

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	ATOM	367	CG	HIS A	117	54.881	26.005	-4.258	1.00 31.82	A
	ATOM	368	CD2	HIS A	117	55.309	27.249	-3.935	1.00 33.19	A
	ATOM	369	ND1	HIS A	117	53.536	25.974	-3.961	1.00 34.30	Α
	ATOM	370	CE1	HIS A	117	53.165	27.148	-3.480	1.00 34.58	Α
5	ATOM	371		HIS A		54.222	27.940	-3.455	1.00 35.18	A
_	ATOM	372	C	HIS A		57.477	24.780	-3.202	1.00 26.22	A
	ATOM	373	ō	HIS A		57.737	25.776	-2.534	1.00 25.67	A
	ATOM	374	N	ILE A		57.469	23.554	-2.689	1.00 24.94	A
	ATOM	375	CA	ILE A		57.792	23.315	-1.285	1.00 23.94	A
10	ATOM	376	СВ	ILE A		57.711	21.812	-0.952	1.00 23.50	A
10	ATOM	377	CG2			58.374	21.533	0.389	1.00 23.76	A
		378		ILE A		56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379		ILE A		56.066	19.858	-0.834	1.00 28.06	A
	MOTA		C	ILE A		59.195	23.821	-0.958	1.00 23.78	A
1.5	MOTA	380			1118		24.495	0.048	1.00 23.49	A
15	ATOM	381	0		1110	60.153	23.489	-1.815	1.00 23.46	A
	MOTA	382	N	ILE A		61.534	23.913	-1.619	1.00 25.13	A
	ATOM	383	CA			62.467	23.250	-2.664	1.00 24.25	A
	ATOM	384	CB	ILE A	1119		23.890	-2.617	1.00 22.47	A
	ATOM	385				63.858	21.738	-2.395	1.00 25.05	A
20	MOTA	386		ILE A		62.540		-3.439	1.00 23.03	A
	MOTA	387		ILE A		63.327	20.945 25.435	-1.705	1.00 25.96	A
	MOTA	388	C		A 119	61.667	26.051	-0.872	1.00 23.30	A
	ATOM	389	0		A 119	62.330		-2.704	1.00 24.70	A
	MOTA	390	N		A 120	61.028	26.039 27.489	-2.704	1.00 27.07	A
25	MOTA	391	CA		A 120	61.100		-4.060	1.00 30.23	A
	MOTA	392	CB		A 120	60.242	27.940	-5.409	1.00 32.34	A
	ATOM	393	CG		A 120	60.674	27.407	-6.512	1.00 35.30	A
	MOTA	394	CD		A 120	59.765	27.950		1.00 46.48	A
	MOTA	395	CE		A 120	58.294	27.636	-6.218	1.00 46.49	A
30	MOTA	396	NZ		A 120	57.363	28.155	-7.252	1.00 40.49	A
	MOTA	397	C		A 120	60.647	28.247	-1.638	1.00 30.89	A
	MOTA	398	0		A 120	61.303	29.198	-1.217	1.00 32.48	A
	MOTA	399	N		A 121	59.527	27.825	-1.055		· A
_	MOTA	400	CA		A 121	58.986	28.488	0.128	1.00 30.33	A
35	MOTA	401	CB		A 121	57.455	28.416	0.117	1.00 35.04	A
	MOTA	402	CG		A 121	56.794	29.021	-1.120		A
	ATOM	403	CD		A 121	57.221	30.456	-1.373	1.00 39.88	A
	MOTA	404		GLU I		57.200	31.264	-0.420	1.00 40.53	A
	ATOM	405		GLU A		57.573	30.778	-2.529	1.00 43.24 1.00 30.37	A
40	MOTA	406	C		A 121	59.511	27.930	1.451		A
	MOTA	407	0		A 121		28.204	2.513	1.00 31.24 1.00 29.03	A
•	MOTA	408	И		A 122	60.588	27.151	1.390	1.00 29.03	A
	MOTA	409	CA		A 122	61.183	26.573	2.594	1.00 28.40	A
	ATOM	410	CB		A 122	61.836	27.673	3.436	1.00 31.28	A
45	MOTA	411	CG		A 122		28.395	2.698		A
	MOTA	412		ASN .				1.754	1.00 35.57	A
	MOTA	413		ASN .			28.169	3.127	1.00 35.73 1.00 26.89	A
	ATOM	414	C		A 122		25.835	3.456		A
	MOTA	415	0		A 122		26.055	4.663	1.00 27.23	A
50	MOTA	416	N		A 123		24.955	2.842	1.00 23.99	A
	MOTA	417	CA		A 123		24.210	3.574	1.00 22.43	A
	MOTA	418	CB		A 123		24.248	2.810	1.00 21.97	A
	MOTA	419	CG		A 123		25.645	2.599	1.00 25.68	A A
	MOTA	420	CD		A 123		26.354	3.927	1.00 27.54	
55	ATOM	421	CE		A 123		27.796	3.716	1.00 31.30	A n
	MOTA	422	NZ		A 123		28.540	5.004	1.00 33.21	A A
	ATOM	423	C		A 123		22.759	3.821	1.00 22.20	A A
	MOTA	424	O		A 123		21.960	4.264	1.00 22.50	A n
	MOTA	425	N	VAL	A 124	59.997	22.412	3.535	1.00 20.59	A

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	ATOM	426	CA	VAL A	124	60.439	21.039	3.730	1.00 20.25	A
	ATOM	427	CB	VAL A		61.922	20.850	3.328	1.00 19.43	A
	ATOM	428		VAL A		62.346	19.407	3.573	1.00 18.69	A
	MOTA	429		VAL A		62.104	21.195	1.853	1.00 18.21	A
5	ATOM	430	C	VAL A		60.236	20.561	5.163	1.00 19.53	A
_	MOTA	431	0	VAL A		59.841	19.418	5.385	1.00 20.02	A
	ATOM	432	N	PRO A		60.513	21.422	6.159	1.00 20.01	A
	ATOM	433	CD	PRO A		61.178	22.738	6.118	1.00 18.69	A
		434	CA	PRO A		60.318	20.979	7.544	1.00 19.88	A
10	ATOM	435	CB	PRO A		60.793	22.180	8.363	1.00 19.95	A
10	ATOM	435	CG	PRO A		61.839	22.805	7.479	1.00 18.85	A
	ATOM		C	PRO A		58.848	20.642	. 7.824	1.00 19.76	A
	ATOM	437	0	PRO A		58.544	19.700	8.550	1.00 16.99	A
	MOTA	438	-			57.947	21.418	7.235	1.00 18.98	A
15	ATOM	439	N	TYR A		56.516	21.220	7.435	1.00 21.97	A
15	ATOM	440	CA	TYR A			22.448	6.933	1.00 25.17	A
	MOTA	441	CB	TYR A		55.752	23.690	7.748	1.00 30.98	A
	ATOM	442	CG	TYR A		56.040	23.886	8.991	1.00 33.95	A
	MOTA	443		TYR A		55.438		9.763	1.00 35.55	A
	MOTA	444	CE1			55.721	25.015		1.00 35.43	A
20	MOTA	445	CD2	TYR A		56.938	24.657	7.292	1.00 33.43	A
	MOTA	446	CE2	TYR A		57.231	25.792	8.058		A
	MOTA	447	CZ	TYR A		56.618	25.962	9.291	1.00 37.40 1.00 40.85	A
	MOTA	448	OH	TYR A		56.903	27.073	10.052	1.00 40.85	A
	MOTA	449	C	TYR A		55.990	19.956	6.762		
25	MOTA	450	0	TYR A		55.265	19.175	7.383	1.00 20.49	A A
	MOTA	451	N	VAL A		56.354	19.746	5.501	1.00 18.16	
	ATOM	452	CA	VAL A		55.892	18.562	4.790	1.00 17.58	A
	MOTA	453	CB	VAL A		56.308	18.596	3.308	1.00 17.45	A
	MOTA	454		VAL A		55.786	17.350	2.600	1.00 17.97	A
30	MOTA	455		VAL A		55.751	19.850	2.641	1.00 14.90	A
	ATOM	456	C	VAL A		56.459	17.306	5.448	1.00 18.39	A
	MOTA	457	0	VAL A		55.769	16.298	5.583	1.00 18.14	A
	MOTA	458	N	THR A		57.716	17.381	5.869	1.00 17.50	A
	MOTA	459	CA	THR A		58.375	16.260	6.530	1.00 18.54	A
35	ATOM	460	CB	THR A		59.861	16.586	6.805	1.00 18.01	A
	ATOM	461	OG1	THR A		60.537	16.804	5.559	1.00 21.14	A
	MOTA	462	CG2			60.536	15.446	7.545	1.00 17.95	A
	MOTA	463	C		128	57.676	15.941	7.856	1.00 19.49	A
	ATOM	464	0		128	57.438	14.776	8.179	1.00 18.76	A
40	ATOM	465	И	ARG A		57.345	16.981	8.619	1.00 19.60	A
	MOTA	466	CA	ARG A	129	56.673	16.804	9.904	1.00 20.12	A
	ATOM	467	CB		129	56.534	18.144	10.621	1.00 21.33	A
	MOTA	468	CG	ARG A	129	55.948	18.029	12.023	1.00 28.02	A
	MOTA	469	CD	ARG A	129	55.721	19.404	12.597	1.00 31.25	A
45	ATOM	470	NE		129	56.940	20.205	12.560	1.00 37.78	A
	ATOM	471	CZ		129	56.962	21.524	12.391	1.00 40.10	A
	ATOM	472	NH1	ARG I	A 129	55.828	22.197	12.239	1.00 40.03	A
	MOTA	473	NH2	ARG A		58.119	22.170	12.374	1.00 44.58	A
	ATOM	474	C	ARG A	A 129	55.288	16.186	9.729	1.00 20.08	A
50	ATOM	475	0	ARG 2	A 129	54.891	15.305	10.496	1.00 20.40	A
	ATOM	476	N	GLU :	A 130	54.553	16.654	8.724	1.00 18.79	A
	MOTA	477	CA		A 130	53.222	16.125		1.00 20.10	A
	MOTA	478	CB	GLU .	A 130	52.638	16.749	7.183	1.00 19.92	A
	ATOM	479	CG	GLU .	A 130	51.350	16.087	6.708	1.00 27.85	A
55	MOTA	480	CD	GLU .	A 130	50.581	16.933	5.707	1.00 29.72	A
	ATOM	4.81	OE1	GLU .	A 130	51.216	17.528	4.814	1.00 33.46	A
	MOTA	482	OE2	GLU.	A 130		16.996	5.807	1.00 30.74	A
	ATOM	483	C	GLU .	A 130	53.301	14.615	8.295	1.00 19.81	A
	MOTA	484	0	GLU .	A 130	52.553	13.875	8.935	1.00 18.37	A

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	MOTA	485	N	ARG A	131	54.219	14.162	7.447	1.00 20.41	A
	ATOM	486	CA	ARG A	131	54.397	12.735	7.202	1.00 22.45	A
	ATOM	487	CB	ARG A	131	55.442	12.511	6.098	1.00 25.16	A
	ATOM	488	CG	ARG A	131	55.742	11.043	5.840	1.00 28.75	A
5	ATOM	489	CD	ARG A	131	56.736	10.837	4.708	1.00 33.75	A
•	ATOM	490		ARG A		57.020		4.520	1.00 40.07	A
	ATOM	491·	_	ARG A		57.756		3.532	1.00 43.07	A
	ATOM	492		ARG A		58.293		2.625	1.00 44.91	Α
	MOTA	493		ARG A		57.955		3.449	1.00 44.45	A
10	ATOM	494	C	ARG A		54.820		8.466	1.00 23.24	Α
10		495	0	ARG A		54.241		8.804	1.00 23.86	A
	MOTA		N	ASP A		55.831		9.160	1.00 21.99	A
	ATOM	496		ASP A		56.318		10.370	1.00 22.04	A
	ATOM	497				57.570		10.888	1.00 23.72	А
	MOTA	498	CB	ASP A		58.750		9.932	1.00 27.77	A
15	MOTA	499	CG	ASP A				8.989	1.00 27.34	A
	MOTA	500		ASP A		58.681		10.128	1.00 28.70	A
	MOTA	501		ASP A		59.753		11.474	1.00 20.70	A
	MOTA	502	C	ASP A		55.258			1.00 22.75	A
	MOTA	503	0	ASP A		55.077		12.092		A
20	MOTA	504	N	VAL A		54.551		11.725	1.00 19.54	A
	ATOM	505	CA	VAL A		53.525		12.759	1.00 18.52	A
•	MOTA	506	CB	VAL A		52.908		12.990	1.00 19.26	
	MOTA	507		VAL A		51.708		13.918	1.00 18.79	A
	MOTA	508	CG2	VAL A		53.953		13.604	1.00 18.80	A
25	MOTA	509	C	VAL A	133	52.419		12.398	1.00 19.46	A
	ATOM	510	0	VAL A	133	52.073		13.200	1.00 19.94	A
	MOTA	511	N	MET A	134	51.878		11.187	1.00 19.15	A
	MOTA	512	CA	MET A	134	50.80	7 11.052	10.792	1.00 21.25	A
	MOTA	513	CB	MET A	134	50.30	9 11.381	9.383	1.00 17.34	A
30	ATOM	514	CG	MET A	134	49.61	12.730	9.302	1.00 20.00	A
	ATOM	515	SD	MET A	134	48.64	3 12.952	7.798	1.00 24.21	A
	ATOM	516	CE	MET A	134	47.03	3 12.434	8.400	1.00 23.20	A
`	MOTA	517	С	MET A	134	51.20	9.582	10.881	1.00 22.43	A
	ATOM	518	0	MET A	134	50.38	4 8.741	11.249	1.00 23.82	A
35	ATOM	519	N	SER A	135	52.45	9.273	10.556	1.00 23.09	A
	ATOM	520	CA	SER A	135	52.93	7.895	10.615	1.00 26.13	A
	ATOM	521	CB	SERA	135	54.35	6 7.798	10.039	1.00 26.17	. A
	ATOM	522	OG	SER A		54.38	3 8.177	8.673	1.00 31.91	A
	ATOM	523	C	SER A	135	52.95	7.358	12.045	1.00 26.58	A
40	ATOM	524	0	SER A	135	52.92	6.148	12.261	1.00 26.42	A
	ATOM	525	N	ARG A		53.01		13.018	1.00 25.65	A
	ATOM	526	CA	ARG A		-53.05	6 7.870	14.425	1.00 27.47	A
	ATOM	527	CB	ARG A		53.82	3 8.914	15.238	1.00 27.97	A
	ATOM	528	CG	ARG A	136	55.28	3 9.082	14.857	1.00 32.00	A
45	ATOM	529	CD	ARG A		55.90		15.664	1.00 33.03	Α
75	MOTA	530	NE	ARG A		55.60		17.084	1.00 36.11	A
	MOTA	531	CZ	ARG A		55.86		18:007	1.00 39.74	A
	ATOM	532		ARG A		56.44		17.661	1.00 40.55	A
	MOTA	533		ARG A		55.54		19.276	1.00 36.72	A
50	ATOM	534	C	ARG A		51.66		15.036	1.00 26.38	A
50		535	ō	ARG A		51.51		16.106	1.00 27.06	A
	MOTA	536	N	LEU A		50.65		14.360	1.00 24.77	A
	ATOM	537	CA	LEU A		49.29		14.870	1.00 24.70	A
	ATOM	53 <i>7</i> 538	CB	LEU A		48.48		14.371	1.00 24.52	A
~~	MOTA	538	CG	LEU A		49.05		14.662	1.00 26.67	A
55	ATOM	540		LEU A		48.07		14.141	1.00 27.25	А
	MOTA			LEU A		49.27			1.00 27.09	A
	ATOM	541				48.59			1.00 25.20	A
	MOTA	542	C	LEU A		48.61			1.00 25.99	A
	MOTA	543	0	LEU A	12/	40.01	. 0.403	13.309	1.00 20.00	-

	ATOM	544	N	ASP	А	138	47.	971	6.218	15.451	1.00	21.89	A
	ATOM	545	CA	ASP	Α	138	47.	239	4.977	15.219	1.00	21.35	A
	ATOM	546	CB	ASP	Α	138	48.	124	3.761	15.523	1.00	22.14	A
	ATOM	547	CG	ASP	Α	138	47.	432	2.448	15.201	1.00	24.90	A
5	ATOM	548	OD1	ASP			46.	631	2.423	14.241	1.00	24.78	A
-	ATOM	549		ASP				691	1.443	15.897	1.00	25.39	A
	ATOM	550	C	ASP				031	4.991	16.138	1.00	20.47	A
	ATOM	551	0	ASP				967	4.248	17.118	1.00	19.06	A
	ATOM	552	N	HIS				075	5.852	15.810		18.27	A
10	ATOM	553	CA	HIS				869	6.016	16.606		18.21	A
10		554	CB	HIS				096	7.157	17.612		15.84	A
	ATOM			HIS				985	7.332	18.600		15.24	A
	MOTA	555	CG					884	6.964	19.900		13.97	A
	MOTA	556		HIS				791	7.943	18.280		14.74	A
1.5	ATOM	557		HIS					7.943	19.341		14.19	A
15	ATOM	558		HIS				002		20.336		14.15	A
	MOTA	559		HIS				641	7.356			18.50	A
	ATOM	560	C	HIS				715	6.330	15.654		20.80	A
	ATOM	561	0	HIS				879	7.080	14.693			A
	ATOM	562	N			140		527	5.767	15.913		18.32	A
20	MOTA	563	CD			140		143	4.984	17.100		16.71	
	MOTA	564	CA			140		367	6.001	15.048		17.43	A
	MOTA	. 565	CB			140		273	5.157	15.704		16.64	A
	ATOM	566	CG			140		643	5.204	17.152		18.43	A
	MOTA	567	С			140		914	7.441	14.803		18.77	A
25	MOTA	568	0			140		207	7.695	13.831		19.88	A
	ATOM	569	N	PHE	Α	141		301	8.381	15.664		17.14	A
	MOTA	570	CA	PHE	Α	141	39.	.874	9.767	15.477		16.42	A
	MOTA	571	CB	PHE	Α	141		. 568	10.422	16.836		14.60	A
	MOTA	572	CG	PHE	Α	141	38.	.386	9.817	17.556		15.26	A
30	MOTA	573	CD1	PHE	A	141	37.	.335	9.234	16.842		14.78	A
	MOTA	574	CD2	PHE	Α	141	38.	.297	9.880	18.942		13.70	A
	MOTA	575	CE1	PHE	Α	141	36.	.215 .	8.727	17.502		16.94	A
	MOTA	576	CE2	PHE	Α	141	37.	.178	9.375	19.615		15.75	A
	MOTA	577	cz	PHE	Α	141	36.	. 135	8.799	18.893		16.89	A
35	MOTA	578	C	PHE	A	141	40.	.857	10.641	14.694		16.15	A
	MOTA	579	0	PHE	Α	141	40	.799	11.871	14.761		17.35	Α
	ATOM	580	N	PHE	Α	142	41	.748	10.011	13.941		15.88	A
	ATOM	581	CA	PHE	Α	142	42	.727	10.756	13.154		17.89	A
	MOTA	582	CB	PHE	Α	142	44	.115	10.645	13.793		17.57	A
40	ATOM	583	CG	PHE	Α	142	44	.240	11.371	15.103	1.00	18.74	A
	MOTA	584	CD1	PHE	Α	142	44	.559	12.726	15.135	1.00	17.77	A
	ATOM	585	CD2	PHE	Α	142	43	.997	10.711	16.304	1.00	18.74	A
	ATOM	586	CE1	PHE	Α	142	44	. 632	13.417	16.347	1.00	15.77	A
	ATOM	587	CE2	PHE	Α	142	44	.065	11.393	17.522	1.00	17.56	A
45	ATOM	588	cz	PHE	Α	142	44	.383	12.747	17.542		17.14	A
	ATOM	589	С			142		. 793	10.231	11.729	1.00	19.12	A
	ATOM	590	0			142	42	.659	9.030	11.504	1.00	20.01	A
	ATOM	591	N			143	42	. 978	11.135	10.769	1.00	18.72	A
	ATOM	592	CA	VAL	Α	143		.102	10.735	9.371	1.00	18.52	A
50	ATOM	593	СВ			143	43	.294	11.961	8.440	1.00	20.66	A
50	ATOM	594		VAL				.843	11.521	7.080	1.00	21.29	A
	ATOM	595		VAL				. 958	12.673	8.252	1.00	22.97	A
	ATOM	596	C			143		.342	9.865	9.330	1.00	18.68	A
	ATOM	597	Ö			143		.355	10.199	9.943		18.42	A
55	ATOM	598	N			144		.259	8.745	8.623	1.00	18.30	A
23	ATOM	599	CA			144		.384	7.824	8.535	1.00	18.78	A
	ATOM	600	CB			144		.889	6.373	8.608		22.27	A
	ATOM	601	CG			144		.017	5.340	8.557		29.72	A
	ATOM	602	CD			144		.491	3.912	8.674		34.16	A
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	ATOM	603	CE	LYS	A	144		46.631	2.896	8.577	1.00 37			A
	ATOM	604	NZ	LYS				46.138	1.484	8.629	1.00 39			A
	ATOM	605	C	LYS	Α	144		46.192	8.002	7.261	1.00 18			A
	MOTA	606	0	LYS	A	144		45.643	8.314	6.200	1.00 18			A
5	MOTA	607	N	LEU				47.502	7.816	7.385	1.00 16			A
	ATOM	608	CA	LEU	A	145		48.411	7.900	6.251	1.00 17			A
	ATOM	609	CB	LEU		145		49.686	8.653	6.641	0.50 18			AC1
	MOTA	610	CG	TEU		145		50.734	8.902	5.549	0.50 20			AC1
	MOTA	611	CD1	LEU		145		51.836	9.799	6.093	0.50 18			AC1
10	MOTA	612	CD2	LEU		145	•	51.317	7.581	5.069	0.50 19		-	AC1
	MOTA	613	C			145		48.739	6.450	5.907	1.00 19			A
	MOTA	614	0	LEU	Α	145		49.451	5.772	6.659	1.00 17			A.
	MOTA	615	И	TYR	A	146		48.215	5.972	4.782	1.00 17			A N
	ATOM	616	CA	TYR	Α	146		48.444	4.593	4.358	1.00 17			A.
15	ATOM	617	CB	TYR	Α	146		47.288	4.098	3.486	1.00 17			A
	MOTA	618	CG	TYR	Α	146		45.981	3.926	4.214	1.00 17			A.
	ATOM	619	CD1	TYR	A	146		45.099	4.995	4.377	1.00 16			A
	MOTA	620	CE1	TYR	Α	146		43.881	4.827	5.039	1.00 17			A
	MOTA	621	CD2	TYR	A	146		45.620	2.686	4.735	1.00 18			A.
20	ATOM	622	CE2			146		44.411	2.506	5.399	1.00 19			A.
	MOTA	623	CZ	TYR	Α	146		43.547	3.576	5.544	1.00 17		•	A A
	MOTA	624	OH			146		42.342	3.376	6.169	1.00 20			A
	ATOM	625	С			146		49.735	4.376	3.582		3.72		A
	MOTA	626	0			146		50.382	3.338	3.715	1.00 19			A
25	ATOM	627	N			147		50.110	5.350	2.765	1.00 1			A
	MOTA	628	CA			147		51.307	5.203	1.952	1.00 1			A
	ATOM	629	CB			147		51.007	4.258	0.783	1.00 1			A
	MOTA	630	CG			147		49.835	4.699	-0.070	1.00 1			A
	MOTA	631				147		49.967	5.752	-0.975	1.00 1			A
30	MOTA	632				147		48.595	4.075	0.053	1.00 1			A
	MOTA	633				. 147		48.886	6.178	-1.742		8.56		A
	MOTA	634	CE2			147		47.503	4.492	-0.710	1.00 1			A
	MOTA	635	ĊZ			147		47.647	5.546	-1.610		7.13		A
	MOTA	636	С			147		51.768	6.533	1.395		4.43		Α
35	MOTA	637	0			147		51.045	7.528	1.452	1.00 1			A
	MOTA	638	N			148		52.981	6.534	0.854	1.00 1			A
	ATOM	639	CA			148		53.541	7.718	0.232 1.197	1.00 1			Α
	MOTA	640	CB			148		54.449	8.531	1.537	1.00 2			A
	ATOM	641	OG:			148		55.605	7.760	2.472	1.00 1			A
40	MOTA	642	CG2			148		53.700	8.897 7.262	-0.946	1.00 2			A
	ATOM	643	С			148		54.386		-0.991	1.00 2			A
	ATOM	644	0			148		54.860	6.124 8.149	-1.916	1.00 1			A
	MOTA	645	N			149		54.543	7.877	-3.073	1.00 1			A
	MOTA	646	CA			149		55.368	6.801	-3.989	1.00 1			A
45	MOTA	647	СВ			149		54.748	7.144	-4.544	1.00 1			A
	MOTA	648	CG			149		53.389 53.262	7.888	-5.712	1.00 1			A
	MOTA	649				149		52.235	6.668	-3.927	1.00 1			A
	MOTA	650				149		52.235	8.149	-6.267	1.00 1			A
	ATOM	651				149		50.972	6.923	-4.470	1.00 1			A
50	MOTA	652				149		50.858	7.663	-5.642	1.00 1			Α
	MOTA	653	CZ			A 149		55.542	9.205	-3.774	1.00 2			Α
	MOTA	654	C			A 149		54.934	10.200	-3.376	1.00 1			A
	MOTA	655	0			A 149		56.398	9.241	-4.782	1.00 1			A
	MOTA	656	N			A 150		56.636	10.481	-5.497	1.00 2			A
55	MOTA	657				A 150		57.659	11.347	-4.739	1.00 2			Α
	ATOM	658				A 150		58.986	10.645	-4.414	1.00 2			A
	MOTA	659				A 150		59.988	11.558	-3.692	1.00 2			A
	MOTA	660				A 150		60.693	12.353	-4.321	1.00 2			A
	MOTA	661	OE	ىلى ب	14 .	A 150		55.55						

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	MOTA	662	NE2	GLN A 150	. 6	0.042	11.449	-2.365	1.00 26.47	A
	ATOM	663	С	GLN A 150	5	7.160	10.203	-6.885	1.00 23.88	A
	ATOM	664	0	GLN A 150	5	7.673	9.118	-7.158	1.00 24.79	A
	MOTA	665	N	ASP A 151.	5	6.987	11.171	-7.774	1.00 25.88	Α.
5	ATOM	666	CA	ASP A 151	5	7.527	11.047	-9.117	1.00 26.49	A
	ATOM	667	_	ASP A 151	5	6.437		-10.199	1.00 24.54	A
	ATOM	668		ASP A 151	5	5.544		-10.064	1.00 24.95	A
	ATOM	669		ASP A 151		6.005	13.379	-9.561	1.00 22.44	A
	ATOM	670	OD2	ASP A 151		4.369		-10.490	1.00 25.72	· A
10	ATOM	671	C	ASP A 151		8.515	12.203	-9.220	1.00 28.63	A A
	ATOM	672	0	ASP A 151		8.890	12.780	-8.194	1.00 27.83 1.00 29.21	A
	ATOM	673	N	ASP A 152		8.934		-10.426 -10.562	1.00 25.21	A
	ATOM	674	CA	ASP A 152		9.907		-12.026	1.00 33.94	A
	MOTA	675	CB	ASP A 152		0.325 1.033		-12.557	1.00 38.88	A
15	ATOM	676	CG	ASP A 152 ASP A 152		1.817		-11.791	1.00 39.67	A
	ATOM	677		ASP A 152 ASP A 152		0.817		-13.738	1.00 41.57	A
	MOTA	678 · 679	C C	ASP A 152		9.487		-10.013	1.00 30.90	A
	MOTA MOTA	680	0	ASP A 152		0.316	15.735	-9.482	1.00 31.69	A
20	ATOM	681	И	GLU A 153		8.207		-10.107	1.00 29.44	A
20	ATOM	682	CA	GLU A 153		7.767	16.632	-9.646	1.00 28.69	A
	ATOM	683	СВ	GLU A 153	5	6.984	17.327	-10.766	1.00 32.90	À
	ATOM	684	CG	GLU A 153	<u> </u>	7.451	16.987	-12.183	1.00 40.57	A
	ATOM	685	CD	GLU A 153	5	6.920		-12.675	1.00 45.78	A
25	MOTA	686	OE1	GLU A 153	<u> </u>	55.682		-12.760	1.00 48.91	A
	ATOM	687	OE2	GLU A 153	į	7.736		-12.979	1.00 48.95	A
	MOTA	688	. C	GLU A 153	į	6.929	16.683		1.00 26.43	A
,	MOTA	689	0	GLU A 153		66.947	17.688		1.00 25.08	A
	MOTA	690	N	LYS A 154		56.205	15.610	_	1.00 22.39	A
30	MOTA	691	CA	LYS A 154		55.318	15.631		1.00 21.43	A A
	MOTA	692	CB	LYS A 154		53.861	15.628		1.00 20.33 1.00 21.92	A
	MOTA	693	CG	LYS A 154		53.505	16.716 16.375		1.00 21.32	A
	MOTA	694	CD	LYS A 154		52.211 51.775		-10.077	1.00 20.04	A
25	MOTA	695	CE	LYS A 154		50.631		-10.951	1.00 19.97	A
35	ATOM	696	NZ	LYS A 154 LYS A 154		55.458	14.522		1.00 20.43	A
	MOTA	697 698	С 0	LYS A 154		55.949	13.426		1.00 21.13	A
	ATOM ATOM	699	N	LEU A 155		54.985	14.832		1.00 19.69	A
	ATOM	700	CA	LEU A 155		54.950	13.900		1.00 19.10	A
40	ATOM	701	CB	LEU A 155		55.362	14.588		1.00 19.65	A
	ATOM	702	CG	LEU A 155		56.740	15.234	-2.129	1.00 21.20	A
	ATOM	703	CD1	LEU A 155		56.848	15.918	-0.770	1.00 23.42	A
•	MOTA	704	CD2	LEU A 155		57.816	14.174	-2.277	1.00 23.08	A
	ATOM	705	C	LEU A 155		53.478	13.507		1.00 18.87	A
45	MOTA	706	0	LEU A 155		52.600	14.348		1.00 18.61	A
	MOTA	707	N	TYR A 156		53.209	12.249		1.00 15.02	A
	MOTA	708	CA	TYR A 156		51.834	11.783		1.00 16.29	A
•	MOTA	709	CB	TYR A 156		51.470	10.769		1.00 14.20 1.00 17.29	A A
	ATOM	710	CG	TYR A 156		51.603	11.273		1.00 17.29	A
50	ATOM	.711		TYR A 156		52.857	11.429 11.884		1.00 18.68	A
	ATOM	712		TYR A 156		52.978	11.588		1.00 16.43	A
	ATOM	713	CD2			50.474 50.583	12.048		1.00 16.31	A
	ATOM	714	CE2	TYR A 156 TYR A 156		51.835	12.192		1.00 18.17	A
55	MOTA MOTA	715		TYR A 156		51.941	12.65		1.00 17.47	A
55	ATOM ATOM	716 717		TYR A 156		51.657	11.108		1.00 16.32	A
	MOTA	717		TYR A 156		52.412	10.19		1.00 16.27	Α
	ATOM	719		PHE A 157		50.678	11.56			A
	ATOM	720		PHE A 157		50.385	10.96		1.00 16.66	A

								•			
	ATOM	721:	СВ		A 157		50.324	12.014	1.629	1.00 16.91	A
	MOTA	722	CG		A 157		51.631	12.708	1.907	1.00 18.96	A
	MOTA	723	CD1	PHE A	A 157		52.821	12.261	1.340	1.00 20.31	A
	ATOM	724	CD2	PHE A	A 157		51.664	13.829	2.732	1.00 21.12	A
5	ATOM	725	CE1	PHE A	A 157		54.025	12.926	1.585	1.00 22.08	A
	ATOM	726	CE2	PHE A	A 157		52,.865	14.500	2.982	1.00 22.18	A
	ATOM	727	CZ	PHE A	A 157		54.045	14.045	2.405	1.00 21.27	A
	MOTA	728	С	PHE A	A 157		49.016	10.308	0.404	1.00 16.52	A
	ATOM	729	0	PHE A	A 157		48.029	10.979	0.110	1.00 17.32	A
10	ATOM	730	N	GLY A	A 158		48.953	9.002	0.644	1.00 15.97	A
	MOTA	731	CA	GLY 2	A 158		47.684	8.299	0.572	1.00 16.13	A
	ATOM	732	С	GLY 3	A 158		47.000	8.383	1.920	1.00 14.94	A
	MOTA	733	0	GLY 2	A 158		47.445	7.756	2.879	1.00 16.28	. A
	ATOM	734	N	LEU 2	A 159		45.915	9.145	1.989	1.00 13.50	A
15	MOTA	735	CA	PEA :	A 159		45.191	9.340	3.241	1.00 15.20	A
	MOTA	736	CB	LEU :	A 159		45.031	10.835	3.517	1.00 14.20	A
	MOTA	737	CG	LEU .	A 159		46.270	11.726	3.385	1.00 19.00	A
	MOTA	738			A 159	•	45.847	13.188	3.477	1.00 17.12	A
	MOTA	739	CD2		A 159		47.275	11.390	4.471	1.00 14.71	A
20	ATOM	740	C		A 159		43.809	8.716	3.232	1.00 15.53	A
	MOTA	741	0		A 159		43.232	8.472	2.177	1.00 16.05	A
	MOTA	742	N		A 160		43.268	8.469	4.418	1.00 15.86	A
	MOTA	743	CA		A 160		41.932	7.917	4.498	1.00 19.01 1.00 22.90	A A
	MOTA	744	CB		A 160		41.566	7.582	5.949		A
25	MOTA	745	OG		A 160		41.901	8.629	6.833	1.00 24.18	A
	MOTA	746	С		A 160		40.987	8.968	3.924	1.00 20.43 1.00 19.96	A
	MOTA	747	0		A 160		41.213	10.173	4.062	1.00 19.30	A
	MOTA	748	N		A 161		39.945	8.508	3.250 2.644	1.00 19.20	A
	MOTA	749	CA		A 161		38.975	9.406	1.332	1.00 20.00	A
30	ATOM	750	CB		A 161		38.471	8.785	0.666	1.00 20.72	A
	ATOM	751	CG		A 161		37.314 37.222	9.502 10.895	0.682	1.00 18.22	` A
	ATOM	752			A 161		36.180	11.557	0.029	1.00 22.24	A
	MOTA	753.			A 161		36.333	8.784	-0.020	1.00 20.53	A
25	ATOM	754	CD2		A 161 A 161		35.287	9.436	-0.678	1.00 24.24	A
35	ATOM	755	CE2		A 161		35.218	10.822	-0.648	1.00 22.32	A
	MOTA	756	CZ		A 161		34.194	11.471	-1.298	1.00 23.03	A
	MOTA	757	OH C		A 161		37.812	9.681	3.598	1.00 20.14	A
	ATOM	758 759	0		A 161		36.959	8.819	3.810	1.00 19.53	A
40	ATOM	760	Ŋ		A 162		37.791	10.880	4.178	1.00 19.92	` A
40	ATOM ATOM	761	CA		A 162		36.721	11.271	5.099	1.00 21.07	A
	ATOM	762	CB		A 162		37.187	12.419	6.002	1.00 19.60	A
	ATOM	763	C		A 162		35.542	11.712	4.238	1.00 22.07	Α
	MOTA	764	Ö		A 162		35.436	12.875	3.860	1.00 20.66	. A
45	ATOM	765	N		A 163		34.653	10.769	3.945	1.00 23.27	A
77	ATOM	766	CA	LYS	A 163		33.503	11.017	3.080	1.00 27.12	· A
	MOTA	767	СВ	LYS	A 163		32.663	9.741	2.963	1.00 29.68	A
	ATOM	768	CG		A 163		33.455	8.524	2.515	1.00 37.67	Α
	ATOM	769	CD		A 163		32.556	7.310	2.321	1.00 42.24	A
50	ATOM	770	CE		A 163		33.373	6.034	2.185	1.00 44.48	A
50	ATOM	771	NZ		A 163		34.143	5.735	3.430	1.00 44.88	A
	ATOM	772	C		A 163		32.581	12.186	3.411	1.00 25.78	A
	ATOM	773	ō		A 163		32.103	12.863	2.506	1.00 26.53	A
	ATOM	774	N		A 164		32.327	12.441	4.689	1.00 24.57	A
55		775	CA		A 164		31.420	13.522	5.033	1.00 23.77	A
	ATOM	776	СВ		A 164		30.610	13.129	6.265	1.00 25.02	A
	ATOM	777	CG		A 164		29.537	12.101	5.932	1.00 27.54	A
	ATOM	778		LASN	A 164		28.772	12.281	4.983	1.00 28.79	A
	MOTA	779			A 164		29.475	11.024	6.704	1.00 27.13	A

	MOTA	780	C	ASN .	A 16	4		31.	999	14.9		5.1		1.00				Α.
	ATOM	781	0	ASN .	A 16	4		31.	306	15.8		5.5		1.00				A N
	MOTA	782	N	GLY				33.		15.0		4.7		1.00				A A
	MOTA	783	CA	GLY				33.		16.4		4.8		1.00				A
5	MOTA	784	C	GLY				34.		17.0		6.1		1.00				A
	MOTA	785	0	GLY				34.		16.3		7.1 6.1		1.00				A
	MOTA	786	И	GLU				34.		18.3		-		1.00				A
	ATOM	787	CA	GLU				34.		19.3		7.3 6.9		1.00				A
	MOTA	788	CB	GLU				35.		20.		6.2		1.00				Α
10	MOTA	789	CG	GLU				36.		20.5		5.5		1.00				A
	MOTA	790	CD	GLU				36.		22.5			389	1.00	-			Α
	MOTA	791		GĹŪ				36.		21.			596	1.00				Α
	MOTA	792		GLU				37.		19.			369	1.00				Α
	ATOM	793	C	GLU				33. 32.		19.			001		22.			A
15	ATOM	794	0	GLU					791	19.			549	1.00				Α
	ATOM	795	N	LEU					813	19.		10.			22.			A
	MOTA	796	CA	LEU					497	19.		12.			22.			Α
	MOTA	797	CB CG	LEU					706	19.		13.			22.			Α
20	MOTA	798 799		LEU					454	19.		13.		1.00	19	. 66		A
20	MOTA	800		LEU					597	19.		14.		1.00	21	.17		Α
	MOTA	801	CDZ	LEU					193	20.		10.		1.00	23	.49		Α
	MOTA	802	0	LEU					047	21.	209	10.	907	1.00	23	.56		Α
	MOTA MOTA	803	N	LEU					960	21.		9.	948	1.00	24	.25		A
25	MOTA	804	CA	LEU			_		473	23.	245	9.	722	1.00	26	. 64		Α
23	MOTA	805	СВ	LEU					560	24.	099	9.	066		25			A
	ATOM	806	CG	LEU				33.	198	25.	546	8.	707	1.00	27	.34		A
	ATOM	807		LEU	A 1	68		32.	718	26.	296	9.	946		26			A
	ATOM	808	CD2	LEU	A 1	68		34.	418	26.	238	8.	119		0 26			A
30	ATOM	809	C	LEU				31.	234	23.	218	8.	829		0 27			A
	ATOM	810	0	LEU	A 1	68		30.	297	23.	989	9.	030		0 26			A
	ATOM	811	N	LYS	A 1	69		31.	233	22.	320		848		0 26			A
	MOTA	812	CA	LYS	A 1	69		30.	.106		210		934		0 27			'A
	MOTA	813	CB		A 1			30.	.324		064		945		0 30			A.
35	MOTA	814	CG	LYS	A 1	69			. 151		854		993		0 32			A A
	MOTA	815	CD	LYS	A 1	69			.407		728		998		0 35			A
	MOTA	816	CE		A 1				.462		372		683		0 38			A
	MOTA	817	NZ		A 1				.622		263		702		0 41 0 28			Α
	MOTA	818	С		A 1				.801		985		682		0 28			Α
40	MOTA	819	0		A 1				.785		608		371		0 26			Α
	MOTA	820	N		A 1				. 826		094		668		0 26			Α
	ATOM	821	CA		A 1				. 624		.791 .476		434 193		0 25			A
	ATOM	822	CB		A 1				.810 .898		300		251		0 26			A
	MOTA	823	CG		A 1						661		790		0 28		•	Α
45	MOTA	824		TYR					.745 .814		.642		839	1.0	0 26	.85		Α
	MOTA	825		L TYR ? TYR					.127		.884		742		0 27			Α
	MOTA	826			A				.209		. 869		792		0 27			Α
	MOTA	827	CE2		. A :				.049		. 254		343	1.0	0 30	0.02		Α
50	MOTA	828 829			A :				.130		.268		382	1.0	0 29	9.23		A
50	ATOM	830	C		A				.229		.918		376	1.0	0 27	7.59		Α
	ATOM	831			A				.045		.122		642	1.0	0 29	9.25		Α
	ATOM ATOM	832			A				.208		.660		. 882	1.0	0 28	3.16		Α
	ATOM	833			Α				.883		.770		. 763	1.0	0 29	9.03		Α
55	MOTA	834			Α:				.151		.435		. 337	1.0	0 27	7.51		Α
55	ATOM	835		2 ILE					.773	25	.705	13	.084	1.0	0 2	7.97		A
	ATOM	836	CG	1 ILE	. A	171			.872	23	.458	13	.272	1.0	0 26	5.70		A
	MOTA	837	CD	1 ILE	. A	171		31	.163	23	. 996	13	. 856	1.0	00 24	4.07	•	A
	ATOM	838		ILE	Α	171		27	.ó94	24	.796	10	. 944	1.0	00 3	1.41		A

	ATOM	839	0	ILE A 171	26.088	25.335	11.407	1.00 31.69	A
	MOTA	840	N	ARG A 172	27.546	25.047	9.719	1.00 33.21	A
	ATOM	841	CA	ARG A 172	26.874	26.000	8.844	1.00 36.54	A
	ATOM	842	СВ	ARG A 172	27.734	26.314	7.616	1.00 37.73	A
5	ATOM	843	CG	ARG A 172	29.057	27.011	7.912	1.00 41.65	A
-	ATOM	844		ARG A 172	29.708	27.492	6.616	1.00 45.29	A
	ATOM	845	NE	ARG A 172	31.037	28.070	6.812	1.00 48.51	A
	ATOM	846	CZ	ARG A 172	31.314	29.059	7.658	1.00 51.53	A
	ATOM	847		ARG A 172	30.355	29.593	8.406	1.00 53.75	A
10	ATOM	848		ARG A 172	32.553	29.526	7.748	1.00 51.21	A
10	ATOM	849	C	ARG A 172	25.528	25.459	8.378	1.00 37.67	A
	MOTA	850	ō	ARG A 172	24.550	26.200	8.288	1.00 39.09	, A
	ATOM	851	N	LYS A 173	25.481	24.163	8.092	1.00 38.44	Α
	ATOM	852	CA	LYS A 173	24.259	23.528	7.619	1.00 39.25	Α
15	ATOM	853	CB	LYS A 173	24.523	22.061	7.272	1.00 41.89	A
13		854	CG	LYS A 173	23.279	21.298	6.830	1.00 45.52	Α
	MOTA	855	CD	LYS A 173	23.557	19.808	6.653	1.00 49.60	Α
	MOTA	856	CE	LYS A 173	24.477	19.530	5.469	1.00 52.63	A
	MOTA		NZ	LYS A 173	23.855	19.894	4.160	1.00 54.61	A
00	MOTA	857		LYS A 173	23.089	23.608	8.595	1.00 39.30	A
20	MOTA	858	C	LYS A 173	21.981	23.960	8.201	1.00 39.62	A
	ATOM	859	0		23.320	23.282	9.863	1.00 37.96	A
	MOTA	860	N	ILE A 174	22.229	23.314	10.833	1.00 37.36	A
	MOTA	861	CA	ILE A 174 ILE A 174	22.223	21.998	11.652	1.00 37.44	A
	MOTA	862	CB			20.802	10.709	1.00 38.37	A
25	ATOM	863	CG2		23.397	21.850	12.532	1.00 37.25	Α
	ATOM	864	CG1		23.355	20.620	13.418	1.00 36.85	Α
	MOTA	865	CD1		22.259	24.492	11.801	1.00 36.71	A
	MOTA	866	C	ILE A 174		24.556	12.724	1.00 38.05	A
	MOTA	867	0	ILE A 174	21.448	25.423	11.592	1.00 35.48	A
30	MOTA	868	N	GLY A 175	23.185	26.585	12.462	1.00 35.29	A
	ATOM	869	CA	GLY A 175	23.265	26.360	13.737	1.00 35.06	A
	ATOM	870	C	GLY A 175	24.053	27.019	13.970	1.00 37.46	A
	ATOM	871	0	GLY A 175	25.066	25.441	14.571	1.00 33.94	A
	MOTA	872	N	SER A 176	23.581 24.253	25.113	15.822	1.00 32.84	Α
35	ATOM	873	CA	SER A 176	23.938	26.155	16.901	1.00 33.54	A
	MOTA	874	CB ·	SER A 176	22.599	26.056	17.347	1.00 34.86	A
	ATOM	875	og	SER A 176	23.796	23.731	16.276	1.00 32.34	A
	ATOM	876	C	SER A 176	22.726	23.263	15.884	1.00 32.82	A
	MOTA	877	0	SER A 176 PHE A 177	24.609	23.085	17.103	1.00 29.39	Α
40	MOTA	878	N		24.313	21.743	17.597	1.00 27.20	A
	MOTA	879	CA	PHE A 177	25.621	20.989	17.865	1.00 26.39	Α
	ATOM	880	CB	PHE A 177 PHE A 177	26.372	20.585	16.622	1.00 26.18	A
	ATOM	881	CG		26.210	21.277	15.426	1.00 25.30	А
	MOTA	882	CD1		27.266	19.516	16.662	1.00 26.05	A
45	MOTA	883		PHE A 177	26.923	20.912	14.290	1.00 26.59	A
	ATOM	884		PHE A 177		19.143	15.532	1.00 26.06	A
•	MOTA	885		PHE A 177	27.986	19.143	14.343	1.00 25.42	A
	MOTA	886	CZ	PHE A 177		21.752	18.884	1.00 27.00	A
	MOTA	887	C	PHE A 177		22.610	19.747	1.00 26.48	A
50	MOTA	888	0	PHE A 177		20.802	19.022	1.00 26.70	Α
	MOTA	889	N	ASP A 178		20.802	20.260	1.00 26.35	A
	MOTA	890	CA	ASP A 178			20.260	1.00 20.33	A
	MOTA	891	CB	ASP A 178		19.773	19.720	1.00 23.30	A
	ATOM	892	CG	ASP A 178				1.00 32.20	Α
55	MOTA	893		ASP A 178			20.014 19.105	1.00 33.21	A
	MOTA	894		2 ASP A 178			21.311	1.00 25.03	A
	MOTA	895	C	ASP A 178				1.00 23.03	A
	ATOM	896	0	ASP A 178	•			1.00 23.60	A
	MOTA	897	И	GLU A 179	. 22.301	20.003	22.332		

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••	ATOM	898	CA	GLU A	179	23.247	19.644	23.619	1.00 25.18	A
	ATOM	899	CB	GLU A	179	22.542	19.770	24.971	1.00 27.60	A
	ATOM	900	CG	GLU A	179	23.324	19.176	26.130	1.00 32.58	A
	MOTA	901	CD	GLU A	179	22.997	19.845	27.449	1.00 35.82	A
5	MOTA	902	OE1	GLU A	179	21.825	20.224	27.645	1.00 35.95	A
	ATOM	903	OE2	GLU A	179	23.912	19.984	28.291	1.00 38.19	A
	ATOM	904	С	GLU A	179	23.808	18.235	23.450	1.00 24.08	A
	ATOM	905	0	GLU A	179	24.977	17.989	23.756	1.00 22.79	A
	ATOM	906	N	THR A	180	22.983	17.316	22.961	1.00 23.36	A
10	MOTA	907	CA	THR A	180	23.412	15.935	22.761	1.00 22.15	A
	MOTA	908	CB	THR A	180	22.224	15.054	22.320	1.00 23.77	A
	MOTA	909	OG1	THR A	180	21.222	15.075	23.341	1.00 26.37	A
	MOTA	910	CG2	THR A	180	22.670	13.616	22.088	1.00 22.66	A
	MOTA	911	С	THR A	180	24.533	15.830	21.724	1.00 22.01	A
15	ATOM	912	0	THR A	180	25.533	15.141	21.944	1.00 19.87	A
	MOTA	913	N	CYS A	181	24.365	16.511	20.596	1.00 21.21	A
	MOTA	914	CA	CYS A	181	25.372	16.480	19.541	1.00 22.22	\mathbf{A}
	ATOM	915	CB	CYS A	181	24.800	17.065	18.250	1.00 24.62	A
	ATOM	916	SG	CYS A	181	23.435	16.080	17.560	1.00 29.50	A
20	ATOM	917	C	CYS A	181	26.633	17.232	19.954	1.00 23.07	A
	MOTA	918	0	CYS A	181	27.746	16.827	19.608	1.00 23.95	A
	MOTA	919	N	THR A	182	26.463	18.325	20.695	1.00 22.76	A
	MOTA	920	CA	THR A	182	27.606	19.103	21.161	1.00 21.49	A
	MOTA	921	CB	THR A	182	27.167	20.346	21.978	1.00 21.37	A
25	MOTA	922	OG1	THR A	182	26.459	21.262	21.134	1.00 22.50	A
	ATOM	923	CG2	THR A	182	28.379	21.046	22.565	1.00 18.36	A
	MOTA	924	C	THR A	182	28.454	18.215	22.071	1.00 21.48	A
•	MOTA	925	0	THR A		29.669	18.090	21.894	1.00 19.95	A
-	MOTA	926	N	ARG A	183	27.798	17.602	23.050	1.00 18.97	A
30	ATOM	927	CA	ARG A	183	28.468	16.723	23.996	1.00 19.39	A
	ATOM	928	CB	ARG	183	27.455	16.140	24.984	0.50 19.46	AC1
	ATOM	929	CG	ARG	183	28.030	15.062	25.887	0.50 18.77	AC1
	ATOM	930	CD	ARG	183	27.021	14.571	26.925	0.50 21.19	AC1
	ATOM	931	NE	ARG	183	26.605	15.642	27.824	0.50 19.46	AC1
35	MOTA	932	CZ	ARG	183	25.496	16.362	27.679	0.50 20.45	AC1
	MOTA	933		ARG	183	24.672	16.123	26.666	0.50 19.81	AC1
	MOTA	934		ARG	183	25.224	17.338	28.539	0.50 17.11	AC1
	MOTA	935	C	ARG A		29.206	15.577	23.302	1.00 20.02	A
	MOTA	936	0	ARG A		30.383	15.333	23.573	1.00 19.97	A
40	ATOM	937	N	PHE A		28.520	14.871	22.409	1.00 19.24	A ·
	ATOM	938	CA	PHE A		29.144	13.746	21.722	1.00 18.04	A
	ATOM	939	CB	PHE A		28.158	13.078	20.764	1.00 21.05	A
-	ATOM	940	CG	PHE A		28.719	11.857	20.098	1.00 22.67	A A
	ATOM	941				28.717	10.630	20.754	1.00 22.97	
45	ATOM	942		PHE A		29.317	11.949	18.850	1.00 19.97	A A
	ATOM	943		PHE A		29.308	9.510	20.176	1.00 23.53	A
	MOTA	944		PHE A		29.915	10.833	18.263	1.00 24.11	
	MOTA	945	CZ	PHE A		29.910	9.613	18.928	1.00 22.97	A A
	MOTA	946	C	PHE A		30.403	14.127	20.941	1.00 17.99 1.00 18.89	A
50	ATOM	947	0	PHE A		31.461	13.531	21.130 20.056	1.00 15.73	A
	ATOM	948	N	TYR A		30.292	15.110		1.00 15.73	A
	ATOM	949	CA	TYR A		31.443	15.519	19.265	1.00 15.72	A
	ATOM	. 950	CB	TYR A		30.992 30.364	16.413	18.111	1.00 17.33	A
	ATOM	951	CG	TYR A			15.584 14.809	17.015 16.168	1.00 19.37	A
55	ATOM	952		TYR A		31.159 30.590	13.952	15.232	1.00 18.12	A
	ATOM	953		TYR A			15.484	16.892	1.00 18.12	A
	MOTA	954 055		TYR A		28.976 28.398	14.623	15.956	1.00 18.90	A
	ATOM	955 056	CEZ	TYR A		29.211	13.861	15.133	1.00 18.41	A
	ATOM	956	CZ	TYR A	182	, 23.211	73.001	T). T)	2.00 10.42	••

	ATOM	957	OH	TYR F	185	28.650	12.995	14.218	1.00 20.48	A
	ATOM	958	С	TYR F	185	32.544	16.172	20.083	1.00 15.79	A
	MOTA	959	0	TYR A	185	33.720	16.015	19.766	1.00 17.69	A
	MOTA	960	N	THR A	186	32.176	16.887	21.142	1.00 15.68	A
5	ATOM	961	CA	THR A	186	33.184	17.504	21.997	1.00 16.03	A
	ATOM	962	CB	THR A	186	32.559	18.403	23.094	1.00 16.62	A
	ATOM	963	OG1	THR A	186	31.866	19.503	22.481	1.00 14.79	A
	ATOM	964	CG2	THR A	186	33.656	18.953	24.019	1.00 14.68	A
	ATOM	965	С	THR A	186	33.954	16.375	22.680	1.00 15.59	A
10	ATOM	966	o	THR A		35.176	16.443	22.823	1.00 13.77	A
	ATOM	967	N	ALA A	187	33.234	15.333	23.097	1.00 14.06	A
	ATOM	968	CA	ALA A		33.869	14.196	23.757	1.00 14.74	Α
•	ATOM	969	CB	ALA A		32.810		24.224	1.00 14.32	A
	ATOM	970	C	ALA A		34.875		22.821	1.00 14.41	A
15	ATOM	971	ō	ALA A		35.972		23.247	1.00 15.61	A
	ATOM	972	N	GLU A		34.51		21.549	1.00 14.01	A
	ATOM	973	CA	GLU A		35.443		20.615	1.00 13.50	A
	ATOM	974	СВ	GLU A		34.782		19.251	1.00 12.85	A
	ATOM	975	CG	GLU A		33.622		19.282	1.00 12.71	A
20	ATOM	976	CD	GLU A		33.464		17.979	1.00 15.01	A
20	ATOM	977	OE1			33.68		16.899	1.00 13.21	A
	ATOM	978	OE2	GLU A		33.11		18.031	1.00 17.69	A
	MOTA	979	C	GLU A		36.682		20.436	1.00 13.34	A
	ATOM	980	Ö	GLU A		37.80		20.408	1.00 14.69	A
25	ATOM	981	N		A 189	36.48		20.326	1.00 13.52	A
23	ATOM	982	CA		A 189	37.62		20.159	1.00 13.35	A
	ATOM	983	CB		1 189	37.16		19.939	1.00 13.95	A
	ATOM	984	CG2	ILE		38.38		19.822	1.00 12.47	A
	ATOM	985		ILE A		36.30		18.671	1.00 13.44	Α
30	ATOM	986	CD1	ILE A		35.58	3 18.664	18.491	1.00 14.29	A
	ATOM	987	С		A 189	38.53		21.394	1.00 14.63	A
	MOTA	988	0	ILE A	A 189	39.75	3 15.595	21.271	1.00 12.97	A
	ATOM	989	N	VAL A	A 190	37.92	7 15.751	22.582	1.00 14.35	A
	ATOM	990	CA	VAL A	A 190	38.68	15.655	23.832	1.00 13.22	Α
35	MOTA	991	CB	VAL Z	A 190	37.74	3 15.690	25.061	1.00 14.28	A
	ATOM	992	CG1	VAL Z	A 190	38.50	9 15.267	26.326	1.00 15.08	A
	MOTA	993	CG2	VAL Z	A 190	37.16	0 17.082	25.233	1.00 12.08	A
	ATOM	994	С	VAL Z	A 190	39.46	8 14.338	23.859	1.00 14.61	A
	ATOM	995	0	VAL Z	A 190	40.63	4 14.304	24.250	1.00 13.72	Α
40	ATOM	996	N	SER A	A 191	38.82	5 13.254	23.432	1.00 15.26	Α
	ATOM	997	CA	SER I	A 191	39.47	8 11.943	23.421	1.00 16.81	A
	ATOM	998	CB	SER	.191	38.47	0 10.857	23.041	0.50 16.14	AC1
	ATOM	999	OG	SER	191	39.01	9.569	23.238	0.50 16.94	AC1
	MOTA	1000	C	SER A	A 191	40.64	9 11.928	22.441	1.00 16.58	A
45	ATOM	1001	0	SER I	A 191	41.69	7 11.335	22.713	1.00 13.96	· A
	ATOM	1002	N		A 192	40.46	B 12.586	21.300	1.00 15.26	A
	ATOM	1003	CA	ALA Z	A 192	41.51	8 12.645	20.292	1.00 14.37	A
	ATOM	1004	CB	ALA I	A 192	40.98	9 13.296	19.016	1.00 14.43	A
	ATOM	1005	C	ALA	A 192	42.69	5 13.440	20.845	1.00 16.46	A
50	MOTA	1006	0	ALA	A 192	43.85	1 13.038	20.697	1.00 17.96	A
	MOTA	1007	N	LEU 2	A 193	42.40	1 14.563	21.496	1.00 15.02	A
	ATOM	1008	CA		A 193	43.45	9 15.392	22.067	1.00 15.42	Α
	ATOM	1009	CB		A 193	42.88	4 16.712	22.600	1.00 12.88	A
	ATOM	1010	CG	LEU 2	A 193	42.44	5 17.721	21.525	1.00 15.97	Α
55	ATOM	1011	CD1	LEU .		41.86	9 18.979	22.190	1.00 13.97	A
	ATOM	1012		LEU .		43.64	2 18.088	20.655	1.00 14.58	A
	ATOM	1013	С	LEU .	A 193	44.21	1 14.659	23.174		Α
	ATOM	1014	0	LEU .	A 193	45.42		23.310	1.00 16.56	A
	MOTA	1015	N	GLU .	A 194	43.50	0 13.870	23.975	1.00 13.96	A

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	ATOM	1016	CA	GLU A	194	44.179	13.123	25.032	1.00 14.08	A
	ATOM	1017	CB	GLU A	194	43.190	12.295	25.857	1.00 14.65	Α
	ATOM	1018	CG	GLU A	194	43.882	11.301	26.789	1.00 17.09	A
	MOTA	1019	CD	GLU A	194	42.924	10.592	27.730	1.00 19.59	A
5	ATOM	1020	OE1	GLU A	194	41.809	10.237	27.295	1.00 19.25	A
	ATOM	1021	OE2	GLU Z	194	43.302	10.380	28.906	1.00 20.20	A
	ATOM	1022	С	GLU A	194	45.208	12.199	24.386	1.00 13.57	A
	ATOM	1023	0	GLU Z	A 194	46.337	12.093	24.847	1.00 14.23	A
	ATOM	1024	N	TYR Z	A 195	44.822	11.544	23.301	1.00 14.89	A
10	ATOM	1025	CA	TYR Z		45.743	10.642	22.618	1.00 16.58	A
_	ATOM	1026	CB	TYR Z	A 195	45.030	9.910	21.488	1.00 17.29	A
	MOTA	1027	CG	TYR I	A 195	45.956	9.058	20.649	1.00 17.92	A
	ATOM	1028	CD1	TYR Z	A 195	46.347	7.788	21.077	1.00 17.96	A
	ATOM	1029		TYR Z		47.203	6.996	20.304	1.00 19.77	A
15	MOTA	1030	CD2	TYR Z	A 195	46.445	9.524	19.428	1.00 16.67	, A
	ATOM	1031	CE2	TYR I		47.299	8.744	18.650	1.00 18.51	Α
	ATOM	1032	CZ		A 195	47.671	7.481	19.094	1.00 20.24	Α
	ATOM	1033	ОН		A 195	48.506	·6.705	18.325	1.00 21.89	Α
	ATOM	1034	С		A 195	46.917	11.419	22.035	1.00 16.98	Α
20	ATOM	1035	ō		A 195	48.081	11.047	22.203	1.00 14.61	A
	ATOM	1036	N		A 196	46.599	12.507	21.347	1.00 16.30	Α
	MOTA	1037	CA		A 196	47.619	13.328	20.720	1.00 18.15	A
	ATOM	1038	CB		A 196	46.969	14.502	19.982	1.00 18.59	A
	ATOM	1039	CG		A 196	47.834	15.203	18.935	1.00 22.51	Α
25	ATOM	1040		LEU		48.222	14.206	17.841	1.00 20.94	A
	ATOM	1041		LEU		47.060	16.375	18.338	1.00 22.98	Ά
	ATOM	1042	C		A 196	48.592	13.844	21.763	1.00 17.75	A
	ATOM	1043	0	LEU	A 196	49.801	13.644	21.649	1.00 18.33	A
	ATOM	1044	N		A 197	48.064	14.495	22.792	1.00 17.12	A
30	ATOM	1045	CA		A 197	48.913	15.042	23.842	1.00 18.47	A
	ATOM	1046	CB		A 197	48.069	15.866	24.817	1.00 15.90	A
	ATOM	1047	CG		A 197	47.571	17.152	24.231	1.00 19.15	A
	ATOM	1048	CD2	HIS	A 197	47.830	17.745	23.038	1.00 18.22	A
	MOTA	1049	ND1	HIS	A 197	46.704	17.992	24.897	1.00 17.47	A
35	ATOM	1050	CE1	HIS	A 197	46.450	19.047	24.139	1.00 19.74	A
	ATOM	1051	NE2	HIS	A 197	47.119	18.921	23.007	1.00 15.69	A
	ATOM	1052	С	HIS	A 197	49.696	13.958	24.572	1.00 19.40	A
	MOTA	1053	0		A 197	50.823	14.192	25.021	1.00 19.42	A
	ATOM	1054	N	GLY	A 198	49.106	12.770	24.679	1.00 18.59	A
40	ATOM	1055	CA	GLY	A 198	49.793	11.675	25.339	1.00 19.60	A
	ATOM	1056	C	GLY	A 198	51.075	11.307	24.612	1.00 21.86	A
	ATOM	1057	0	GLY	A 198	51.963	10.682	25.186	1.00 23.09	A
	ATOM-	1058	N	LYS	A 199	51.174	11.687	23.341	1.00 22.81	A
	MOTA	1059	CA	LYS	A 199	52.368	11.401	22.549	1.00 24.43	A
45	ATOM	1060	CB	LYS	A 199	51.990	10.905	21.154	. 1.00 26.00	Α
_	ATOM	1061	CG	LYS	A 199	51.378	9.520	21.133	1.00 30.98	A
	ATOM	1062	CD		A 199		9.002	19.708	1.00 36.85	A
	ATOM	1063	CE	LYS	A 199	50.832	7.559	19.682	1.00 40.37	A
	ATOM	1064	NZ	LYS	A 199	51.646	6.691	20.581	1.00 43.48	A
50	ATOM	1065	C	LYS	A 199	53.253	12.631	22.414	1.00 23.88	A
	ATOM	1066	0	LYS	A 199	54.144	12.669	21.568	1.00 24.97	A
	MOTA	1067	N	GLY	A 200	52.997	13.638	23.243	1.00 24.00	Α
	MOTA	1068	CA	GLY	A 200	53.790	14.853	23.203	1.00 22.12	Α
	MOTA	1069	C	GLY	A 200	53.665	15.632	21.907	1.00 22.14	A
55	MOTA	1070	0	GLY	A 200	54.632	16.231	21.439	1.00 22.41	A
	MOTA	1071	N	ILE	A 201	52.475	15.630	21.320	1.00 20.00	A
	MOTA	1072	CA	ILE	A 201		16.355	20.080	1.00 18.93	A
	ATOM	1073	CB	ILE	A 201	51.784	15.414	18.955	1.00 19.70	A
	MOTA	1074	CG2	: ILE	A 201	51.414	16.226	17.716	1.00 20.12	A

	ATOM	1075	CG1	ILE A	201	52.880	14.395	18.636	1.00 20.03	A
	MOTA	1076		ILE A		52.408	13.258	17.745	1.00 22.75	A
	MOTA	1077	C	ILE A		51.193	17.425	20.270	1.00 19.87	A
	ATOM	1078	ō	ILE A		50.121	17.161	20.817	1.00 20.08	A
5	ATOM	1079	N	ILE A		51.508	18.633	19.815	1.00 19.94	A
,	ATOM	1080	CA	ILE A		50.601	19.772	19.891	1.00 20.45	A
	ATOM	1081	CB	ILE A		51.352	21.040	20.356	1.00 22.21	A
	ATOM	1082		ILE A		50.381	22.220	20.470	1.00 22.67	A
	ATOM	1083		ILE A		52.033	20.775	21.700	1.00 24.19	A
10	ATOM	1084		ILE A		52.914	21.920	22.169	1.00 25.39	A
10	ATOM	1085	C	ILE A		50.105	19.999	18.464	1.00 20.71	A
	ATOM	1086	ō	ILE A		50.910	20.067	17.538	1.00 19.48	A
	ATOM	1087	N	HIS A		48.795	20.108	18.270	1.00 18.65	A
	ATOM	1088	CA	HIS A		48.280	20.319	16.919	1.00 18.02	A
15	ATOM	1089	CB	HIS A		46.775	20.057	16.874	1.00 16.31	A
13	MOTA	1090	CG	HIS A		46.199	20.136	15.495	1.00 18.36	A
	ATOM	1091		HIS A		46.043	21.186	14.655	1.00 16.42	A.
	ATOM	1092		HIS A		45.759	19.026	14.806	1.00 19.50	A
	ATOM	1093		HIS A		45.359	19.389	13.600	1.00 17.64	A
20	ATOM	1094		HIS A		45.522	20.694	13.483	1.00 20.87	A
20	MOTA	1095	C	HIS A		48.589	21.738	16.405	1.00 18.92	A
	ATOM	1096	ō	HIS A		49.073	21.906	15.282	1.00 16.21	A
	ATOM	1097	N	ARG A		48.301	22.744	17.232	1.00 18.60	A
	ATOM	1098	CA	ARG A		48.552	24.157	16.914	1.00 19.81	A
25	ATOM	1099	CB	ARG A		49.998	24.365	16.458	1.00 21.61	A
	ATOM	1100	CG	ARG A	204	51.024	24.137	17.550	1.00 23.82	A
	MOTA	1101	CD	ARG A	204	52.323	24.870	17.252	1.00 27.62	A
	MOTA	1102	NE	ARG A	204	52.932	24.449	15.994	1.00 29.43	A
	ATOM	1103	CZ	ARG A	204	54.125	24.861	15.572	1.00 33.10	A
30	MOTA	1104	`NH1	ARG A	204	54.835	25.706	16.311	1.00 32.12	A
	MOTA	1105	NH2	ARG A	204	54.614	24.426	14.418	1.00 30.25	. A
	ATOM	1106	С	ARG A	204	47.624	24.830	15.905	1.00 20.03	^ A
	MOTA	1107	0	ARG A	204	47.711	26.038	15.698	1.00 20.88	A
	MOTA	1108	N ·	ASP A	205	46.755	24.071	15.255	1.00 18.96	A
35	MOTA	1109	CA	ASP A	205	45.828	24.692	14.325	1.00 17.90	A
	ATOM	1110	CB	ASP A		46.418	24.741	12.914	1.00 18.95	A
	ATOM	1111	CG	ASP A		45.655	25.688	12.008	1.00 20.36	A A
	MOTA	1112		. ASP A		44.939	26.560	12.545	1.00 20.35	A
	MOTA	1113		ASP A		45.772	25.573	10.771	1.00 22.49 1.00 19.60	A
40	ATOM	1114	C		205	44.500	23.956	14.328	1.00 19.50	A
	MOTA	1115	0		A 205	43.876	23.751	13.287	1.00 21.53	A
	ATOM	1116	N		A 206	44.063	23.569	15.521 15.667	1.00 10.33	A
	MOTA	1117	CA		A 206	42.813	22.851 22.295	17.087	1.00 18.94	A
	MOTA	1118	CB		A 206	42.693	21.358	17.346	1.00 23.10	A
45	ATOM	1119	CG		A 206	41.511 41.615	20.142	16.436	1.00 23.10	A
	ATOM	1120		L LEU A			20.142	18.808	1.00 23.02	A
	MOTA	1121		LEU A		41.504 41.639	23.772	15.361	1.00 19.05	A
	MOTA	1122	C		A 206 A 206	41.556	24.880	15.886	1.00 19.25	A
50	ATOM	1123	0		A 207	40.740	23.307	14.500	1.00 17.54	A
50	ATOM	1124 1125	N		A 207	39.564	24.081	14.110	1.00 18.60	A
	ATOM ATOM	1125	CA CB		A 207	39.980	25.248	13.196	1.00 18.98	A
	ATOM	1126	CG		A 207	40.786	24.817	11.982	1.00 18.20	\mathbf{A}^{l}
	ATOM	1128	CD		A 207	41.246	26.000	11.139	1.00 21.42	A
55	ATOM	1128	CE		A 207		25.537	10.062	1.00 23.21	A
23	ATOM	1130	NZ		A 207		26.604	9.084	1.00 29.61	A
	ATOM	1131			A 207		23.181	13.388	1.00 18.18	A
	ATOM	1132	ō		A 207		22.100	12.915	1.00 18.11	A
	MOTA	1133			A 208		23.614	13.293	1.00 20.26	A

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1.00 18.79 36.713 24.833 13.882 Α PRO A 208 MOTA 1134 CD 12.616 1.00 19.67 A PRO A 208 36.272 22.814 ATOM 1135 CA 23.742 12.608 1.00 19.45 Α СВ PRO A 208 35.063 MOTA 1136 1.00 21.81 MOTA 1137 CG PRO A 208 35.231 24.509 13.891 Α 1.00 21.04 11.209 Α PRO A 208 36.674 22.372 MOTA 1138 C 10.751 1.00 21.19 Α 36.264 21.307 ATOM 1139 0 PRO A 208 1.00 21.69 GLU A 209 37.474 23.188 10.528 Α ATOM 1140 N 9.170 1.00 22.64 Α **GLU A 209** 37.928 22.872 CA ATOM 1141 0.50 23.65 AC1 38.644 24.084 8.558 CB GLU 209 MOTA 1142 . AC1 0.50 27.24 10 209 39.253 23.825 7.185 MOTA 1143 CG GLU 40.155 24.958 6.716 0.50 29.40 AC1 MOTA 1144 CD GLU 209 0.50 29.68 AC1 39.660 26.094 6.553 209 OE1 GLU MOTA 1145 AC1 OE2 GLU 209 41.363 24.711 6.511 0.50 30.07 MOTA 1146 1.00 22.28 Α 9.159 **GLU A 209** 38.879 21.668 MOTA 1147 C 8.170 1.00 21.36 Α 20.933 15 MOTA 1148 **GLU A 209** 38.955 0 ASN A 210 39.600 21.490 10.263 1.00 19.90 Α ATOM 1149 N 10.436 1.00 19.44 Α 40.574 20.412 MOTA 1150 CA ASN A 210 Α 41.744 20.912 11.287 1.00 20.07 CB **ASN A 210** MOTA 1151 1.00 25.77 Α 42.746 21.698 10.479 MOTA 1152 CG **ASN A 210** 11.029 1.00 26.73 Α 43.571 22.427 20 ATOM 1153 OD1 ASN A 210 42.687 21.548 9.158 1.00 25.15 А ND2 ASN A 210 ATOM 1154 ASN A 210 40.005 19.151 11.078 1.00 18.63 Α MOTA 1155 С 1.00 18.29 40.712 18.154 11.234 Α MOTA 1156 0 ASN A 210 11.469 1.00 16.31 Α ILE A 211 38.739 19.202 ATOM 1157 Ñ 12.085 1.00 15.49 Α 25 38.090 18.058 MOTA 1158 CA ILE A 211 ILE A 211 37.336 18.488 13.354 1.00 15.40 MOTA 1159 CB 36.582 17.311 13.950 1.00 14.59 Α MOTA 1160 CG2 ILE A 211 14.365 1.00 15.91 Α 38.342 19.046 ATOM 1161 CG1 ILE A 211 15.590 1.00 15.98 Α 19.669 37.720 ATOM 1162 CD1 ILE A 211 11.059 1.00 17.26 10.926 1.00 18.16 37.131 17.485 11.059 Α ILE A 211 30 MOTA 1163 C ILE A 211 Α 35.995 17.947 MOTA 1164 0 1.00 15.97 37.599 ATOM 1165 N LEU A 212 16.486 10.317 Α 1.00 17.08 Α 9.274 MOTA 1166 CA **LEU A 212** 36.784 15.875 8.202 1.00 17.78 Α 37.685 15.249 MOTA 1167 CB LEU A 212 7.640 1.00 18.92 38.785 16.157 LEU A 212 35 ATOM 1168 CG 39.476 15.450 6.485 1.00 22.09 Α MOTA 1169 CD1 LEU A 212 17.482 7.166 1.00 19.91 Α ATOM 1170 CD2 LEU A 212 38.188 9.837 1.00 18.35 Α 35.843 14.825 MOTA 1171 C LEU A 212 35.957 14.433 11.002 1.00 19.39 Α LEU A 212 MOTA 1172 0 14.368 9.000 1.00 17.84 Α 40 ATOM 1173 N LEU A 213 34.915 1.00 19.94 33.942 13.362 9.403 Α ATOM 1174 CA LEU A 213 9.487 1.00 20.84 Α ATOM LEU A 213 32.556 14.004 1175 CB 15.059 10.583 1.00 20.31 Α ATOM 1176 CG LEU A 213 32.396 10.367 1.00 22.75 Α 31.124 15.837 CD1 LEU A 213 MOTA 1177 32.379 14.378 11.940 1.00 23.93 Α MOTA 1178 CD2 LEU A 213 45 8.426 1.00 20.98 Ά ATOM 1179 C LEU A 213 33.914 12.187 33.743 12.379 7.218 1.00 19.55 Α MOTA 1180 0 LEU A 213 MOTA ASN A 214 34.088 10.970 8.935 1.00 20.44 Α 1181 N 34.055 8.049 1.00 23.77 Α ATOM 1182 CA ASN A 214 9.814 1.00 25.30 Α MOTA 34.745 8.596 8.674 50 1183 CB ASN A 214 1.00 32.04 Α 34.077 8.127 9.948 ATOM 1184 ASN A 214 CG 32.908 8.422 10.206 1.00 34.43 ATOM 1185 OD1 ASN A 214 34.818 7.369 10.752 1.00 33.85 Α MOTA ND2 ASN A 214 1186 1.00 24.07 Α 32.618 9.466 7.693 MOTA 1187 C ASN A 214 1.00 19.94 Α 10.113 8.150 31.672 ATOM 1188 0 ASN A 214 32.459 6.879 1.00 25.77 GLU A 215 8.433 MOTA 1189 N 1.00 28.69 MOTA 1190 CA GLU A 215 31.138 8.003 6.445 1.00 31.98 31.275 6.796 5.513 MOTA CB GLU A 215 1191 29.970 1.00 40.22 · ATOM 1192 CG GLU A 215 6.334 4.896

	ATOM	1193	CD	GLU A	215		30.182	5.312	3.795	1.00 44.27	A
	MOTA	1194	OE1	GLU A			30.817	4.268	4.065	1.00 46.46	A
	ATOM	1195		GLU A			29.716	5.556	2.660	1.00 46.13	A
	ATOM	1196	С	GLU A			30.188	7.673	7.601	1.00 28.41	A
5	ATOM	1197	0	GLU A	215		28.971	7.769	7.447	1.00 28.52	A
•	ATOM	1198	И	ASP A	216		30.737	7.287	8.752	1.00 26.77	A
	MOTA	1199	CA	ASP A	216		29.914	6.953	9.917	1.00 27.28	A
	ATOM	1200	СВ	ASP A			30.538	5.795	10.696	1.00 31.27	A
	MOTA	1201	CG	ASP A	216		30.390	4.466	9.979	1.00 37.61	A
10	ATOM	1202	OD1	ASP A	216		29.274	4.170	9.499	1.00 39.45	A
-	ATOM	1203		ASP A			31.382	3.710	9.902	1.00 41.84	A
	ATOM	1204	С	ASP A	216		29.697	8.135	10.862	1.00 26.37	A
	ATOM	1205	0	ASP A	216		29.136	7.984	11.950	1.00 25.73	A
	ATOM	1206	N	MET A	217		30.156	9.306	10.441	1.00 23.02	A
15	ATOM	1207	CA	MET A	217		30.015	10.527	11.218	1.00 21.83	A
	ATOM	1208	СВ	MET A	217		28.537	10.789	11.517	1.00 23.24	A
	ATOM	1209	CG	MET A	.217		27.742	11.186	10.274	1.00 22.98	A
	MOTA	1210	SD	MET A	217		28.464	12.616	9.43.0	1.00 27.57	A
	MOTA	1211	CE	MET A	217		27.679	13.974	10.332	1.00 26.68	A
20	MOTA	1212	C	MET A	217		30.844	10.618	12.502	1.00 21.51	A
	MOTA	1213	0	MET A	217		30.474	11.323	13.440	1.00 18.62	A
	ATOM	1214	N	HIS A	218		31.957	9.892	12.544	1.00 20.10	A
	ATOM	1215	CA	HIS A	218		32.873	9.964	13.678	1.00 19.86	A
	ATOM	1216	CB	HIS A	218		33.482	8.594	13.977	1.00 20.21	A
25	MOTA	1217	CG	HIS A			32.551	7.667	14.698	1.00 22.40	A
	MOTA	1218		HIS A			31.910	6.547	14.287	1.00 21.27	A
	ATOM	1219		HIS A			32.177	7.863	16.011	1.00 19.59	A
	MOTA	1220		HIS A			31.348.		16.379	1.00 21.88	A
	MOTA	1221		HIS A			31.168	6.091	15.351	1.00 22.08 1.00 19.10	A A
30	MOTA	1222	C	HIS A			33.947	10.921	13.172	1.00 19.10	A
	ATOM	1223	0	HIS A			34.170	11.004	11.965 14.067	1.00 20.31	A
	MOTA	1224	N	ILE A			34.617	11.638 12.586	13.618	1.00 17.21	A
	ATOM	1225	CA	ILE A			35.628 35.987	13.614	14.716	1.00 15.38	A
2.5	ATOM	1226	CB	ILE A			34.722	14.305	15.221	1.00 14.58	A
35	ATOM	1227		ILE A			36.734	12.919	15.864	1.00 14.46	A
	MOTA	1228 1229		ILE A			37.279	13.885	16.911	1.00 13.74	A
	ATOM		CDI	ILE A			36.929	11.944	13.161	1.00 16.21	A
	ATOM ATOM	1230 1231	0	ILE A			37.238	10.799	13.500	1.00 15.88	A
40	ATOM	1232	И	GLN A			37.677	12.711	12378	1.00 15.62	A
40	ATOM	1233	CA	GLN A			38.980	12.316	11.876	1.00 17.84	A
	ATOM	1234	CB	GLN A			38.872	11.595	10.525	1.00 20.00	A
	ATOM	1235	CG	GLN A			38.463	10.129	10.659	1.00 26.97	A
	ATOM	1236	CD	GLN A			38.648	9.343	9.372	1.00 29.95	A
45	ATOM	1237		GLN A			37.968	9.590	8.373	1.00 33.12	A
	ATOM	1238		GLN F			39.578	8.393	9.389		A
	ATOM	1239	C	GLN A			39.757	13.610	11.735	1.00 17.00	A
	ATOM	1240	0	GLN F	220		39.609	14.339	10.751	1.00 18.27	A
	ATOM	1241	N	ILE A	221		40.566	13.906	12.746	1.00 14.34	. A
50	ATOM	1242	CA	ILE A	221		41.361	15.120	12.753	1.00 14.46	A
	MOTA	1243	CB	ILE A			41.867		14.175	1.00 12.30	A
	MOTA	1244	CG2				42.764		14.167	1.00 14.78	A
	MOTA	1245		L ILE A			40.660		15.102	1.00 13.92	A
	MOTA	1246	CD1	L ILE A			41.003		16.543	1.00 15.06	A.
55	ATOM	1247	C		A 221		42.536		11.783	1.00 15.44	· A
	MOTA	1248	0		A 221		43.106		11.613	1.00 13.93	A
	ATOM	1249	N		A 222		42.877				A
	MOTA	1250	CA		A 222		43.980				A
	MOTA	1251	CB	THR I	A 222	•	43.470	15.836	8.750	1.00 13.32	A

	ATOM	1252	OG1	THR A	222	44.	587	15.637	7.875	1.00		A
	MOTA	1253	CG2	THR A	1 222	42.	630	17.018	8.257	1.00		A
	MOTA	1254	С	THR A	1 222	44.	735	17.428	10.192	1.00		Α
	ATOM	1255	0	THR A	1 222	44.	509	18.257	11.084		18.59	A
5	ATOM	1256	N	ASP A	1 223	45.	630	17.610	9.216		18.69	A
	MOTA	1257	CA	ASP A	1 223	46.	440	18.825	9.069	1.00		A
	MOTA	1258	CB	ASP 7	A 223	45.	532	20.065	9.108		23.51	A
	ATOM	1259	CG	ASP A	A 223	46.	248	21.335	8.670		27.09	A
	MOTA	1260		ASP A		47.	283	21.227	7.975		26.28	A
10	MOTA	1261	OD2	ASP A	A 223		765	22.438	9.009		26.15	A
	MOTA	1262	C		A 223		516	18.913	10.150		21.73	A
	MOTA	1263	0		A 223		439	19.751	11.055		22.76	A
	MOTA	1264	N		A 224		535	18.063	10.027		20.75	A
	MOTA	1265	CA		A 224		611	17.988	11.009		20.11	A
15	MOTA	1266	CB		A 224		805	16.527	11.424		20.62	A
	ATOM	1267	CG		A 224		682	15.991	12.263		21.41	A A·
	MOTA	1268		PHE			598	16.312	13.614		23.05 22.27	A
	MOTA	1269		PHE			681	15.212	11.693		23.30	A
	MOTA	1270		PHE			.528	15.868	14.389		21.11	Ä
20	MOTA	1271	CE2				606	14.763	12.457		22.02	A
	ATOM	1272	CZ		A 224		.530	15.093	13.807		20.45	A
	MOTA	1273	C		A 224		. 957	18.583	10.619 11.407		20.73	A
	MOTA	1274	0		A 224		.905	18.547 19.125	9.412		22.02	A
~-	MOTA	1275	N		A 225		.049	19.713	8.981		22.66	A
25	MOTA	1276	CA		A 225		.301	20.822	9.920		24.99	A
	ATOM	1277	C	•	A 225		.742 .939	20.022	10.122		24.52	A
	ATOM	1278	0		A 225 A 226		.779	21.524	10.508		23.50	A
	ATOM	1279	N		A 226		.106	22.613	11.416		25.16	Α
20	MOTA	1280	CA CB		A 226		.199	23.829	11.160		24.76	A
30	ATOM	1281 1282		THR			.831	23.410	11.113		22.68	A
	ATOM ATOM	1283	CG2		A 226		.571	24.490	9.834		25.00	A
	ATOM	1284	C		A 226		.046	22.233	12.894	1.00	25.79	Α
	ATOM	1285	0		A 226		.019	23.100	13.768	1.00	24.54	A
35	ATOM	1286	N .		A 227		.037	20.935	13.173	1.00	24.97	A
55	MOTA	1287	CA		A 227		.004	20.475	14.550	1.00	25.49	A
	ATOM	1288	CB		A 227		.659	18.993	14.607	1.00	22.85	A
	ATOM	1289	C		A 227		.384	20.715	15.149	1.00	27.70	A
	ATOM	1290	0		A 227	54	.331	21.047	14.435	1.00	26.60	A
40	ATOM	1291	N	LYS	A 228	53	.491	20.558	16.461	1.00	28.53	Α
	ATOM	1292	CA	LYS	A 228	54	.760	20.745	17.149	1.00	32.12	A
	ATOM	1293	CB	LYS	A 228	54	.699	21.974	18.054	1.00	33.81	A
	ATOM	1294	CG	LYS	A 228	56	.007	22.294	18.765		41.23	A
	ATOM	1295	CD	LYS	A 228	57	.082	22.725	17.768		47.57	A
45	MOTA	1296	CE	LYS	A 228	58	.401	23.056	18.462		49.82	A
	MOTA	1297	NZ	LYS	A 228		.459	23.425	17.480		51.49	A
	MOTA	1298	С	LYS	A 228		.019	19.504	17.985		33.25	A
	MOTA	1299	0		A 228	54	.190	19.129	18.815		33.70	Ą
	MOTA	1300	N		A 229		.159	18.860	17.756		33.64	. A
50	MOTA	1301	CA		A 229		.516	17.661	18.501		34.66	A
	MOTA	1302	CB		A 229		.248	16.646	17.609		33.50	A A
	MOTA	1303			A 229		.619	15.419	18.415		32.34	A
•	MOTA	1304			A 229		.370	16.264	16.436		34.25 37.57	A
	ATOM	1305	C		A 229		.420	18.035	19.668		37.57	A
55	ATOM	1306	0		A 229		.581	18.392	19.474		40.57	A
	MOTA	1307	N		A 230		.877	17.948	20.878		46.10	A
	ATOM	1308	CA		A 230		.615	18.289	22.088		44.71	A
	ATOM	1309	CB		A 230		.654	18.417 19.545	23.270	1.00	44.50	A
	ATOM	1310	CG	UHU	A 230	22	.627	エフ・コせコ	23.207	1.00		

	ATOM	1311	CD1	LEU A 230	54.673	19.430	24.383	1.00 44.39	A
	ATOM	1312	CD2	LEU A 230	56.340	20.885	23.214	1.00 44.81	A
	ATOM	1313	С	LEU A 230	58.695	17.279	22.440	1.00 50.42	A
	ATOM	1314	0	LEU A 230	58.603	16.104	22.089	1.00 51.64	A
5	ATOM	1315	N	SER A 231	59.717	17.756	23.145	1.00 55.81	A
_	ATOM	1316	CA	SER A 231	60.824	16.914	23.583	1.00 61.14	A
	ATOM	1317	СВ	SER A 231	62.077	17.200	22.750	1.00 61.27	A
	ATOM	1318	OG	SER A 231	62.444	18.568	22.823	1.00 62.85	A
	ATOM	1319	С	SER A 231	61.124	17.126	25.071	1.00 64.65	A
10	MOTA	1320	0	SER A 231	61.392	16.164	25.794	1.00 65.70	A
	ATOM	1321	N	PRO A 232	61.081	18.387	25.549	1.00 67.54	A
	ATOM	1322	CD	PRO A 232	60.854	19.651	24.823	1.00 68.60	A
	ATOM	1323	CA	PRO A 232	61.358	18.655	26.966	1.00 68.74	A
	ATOM	1324	CB	PRO A 232	61.109	20.158	27.086	1.00 68.83	A A
15	ATOM	1325	CG	PRO A 232	61.505	20.666	25.737	1.00 68.96	A
	MOTA	1326	C	PRO A 232	60.460	17.846	27.899	1.00 69.17 1.00 69.94	A
	MOTA	1327	0	PRO A 232	59.335	17.494	27.541	1.00 80.06	A
	MOTA	1328	N	ALA A 237	57.424	23.198	27.637	1.00 79.29	A
	MOTA	1329	CA	ALA A 237	56.783	23.047	26.335	1.00 78.64	A
20	MOTA	1330	CB	ALA A 237	55.275	22.907	26.512 25.433	1.00 78.04	A
	MOTA	1331	C	ALA A 237	57.092	24.239	25.249	1.00 79.47	A
	ATOM	1332	0	ALA A 237	56.250 58.297	25.113 24.280	24.871	1.00 78.57	A
	ATOM	1333	N	ALA A 238	58.683	25.383	23.992	1.00 78.50	A
	ATOM	1334	CA	ALA A 238 ALA A 238	60.186	25.347	23.728	1.00 78.50	A
25	ATOM	1335	CB	ALA A 238	57.920	25.327	22.673	1.00 78.15	A
	ATOM	1336	C	ALA A 238	57.243	24.341	22.375	1.00 77.96	A
	MOTA	1337 1338	Ŋ	ALA A 239	58.027	26.393	21.887	1.00 77.28	A
	MOTA	1339	CA	ALA A 239	57.338	26.452	20.603	1.00 76.27	A
30	ATOM ATOM	1340	CB	ALA A 239	55.849	26.489	20.827	1.00 76.61	A
30	ATOM	1341	C	ALA A 239	57.766	27.667	19.793	1.00 75.38	A
	MOTA	1342	o	ALA A 239	58.955	27.955	19.700	1.00 75.89	Α
	ATOM	1343	N	ASN A 240	56.781	28.357	19.214	1.00 73.95	Α
	ATOM	1344	CA	ASN A 240	56.967	29.553	18.389	1.00 71.07	A
35	ATOM	1345	СВ	ASN A 240	58.151	30.400	18.874	1.00 71.47	A
-	ATOM	1346	CG	ASN A 240	59.459	30.055	18.174	1.00 72.06	A
	ATOM	1347	OD1	ASN A 240	59.575	30.149	16.943	1.00 72.03	A
	ATOM	1348	ND2	ASN A 240	60.470	29.665	18.964	1.00 71.91	A
	MOTA	1349	С	ASN A 240	57.188	29.178	16.928	1.00 69.41	A
40	MOTA	1350	0	ASN A 240	57.480	28.024	16.624	1.00 70.09	A
	ATOM	1351	N	ALA A 241	57.055	30.165	16.038	1.00 66.62	A
	MOTA	1352	CA	ALA A 241	57.246	30.013	14.585	1.00 63.94	A
	MOTA	1353	C	ALA A 241	55.952	30.080	13.772	1.00 60.63	A n
	MOTA	1354	0	ALA A 241	55.840	30.880	12.845	1.00 61.29	A
45	MOTA	1355	CB	ALA A 241	57.979	28.704	14.246	1.00 65.23	A A
	MOTA	1356	N	PHE A 242	54.984	29.236	14.113	1.00 56.72 1.00 52.53	Ā
	MOTA	1357	CA	PHE A 242	53.712	29.196	13.394	1.00 32.33	A
	MOTA	1358	CB	PHE A 242	53.419	27.767 27.590	12.923 12.354	1.00 47.38	A
	ATOM	1359	CG	PHE A 242	52.040	28.067	11.085	1.00 47.69	A
50	ATOM	1360		1 PHE A 242	51.731	26.975	13.102	1.00 45.45	A
	MOTA	1361		2 PHE A 242	51.038	27.937	10.565	1.00 45.45	A
	MOTA	1362		1 PHE A 242	50.445 49.751	26.840	12.594	1.00 45.41	A
	MOTA	1363		PHE A 242	49.453	27.323	11.322	1.00 46.55	A
<i></i>	MOTA	1364 1365		PHE A 242	52.534	29.688	14.229		A
55	MOTA	1365		PHE A 242	52.502	29.505	15.444		A
	MOTA MOTA	1367		VAL A 243	51.566	30.305			A
	MOTA	1368		VAL A 243	50.355	30.809		1.00 46.21	A
	MOTA	1369		VAL A 243	50.340	32.352			A
	71.011	2000			-				

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	MOTA	1370		VAL				49.012	32.844	14.825	1.00 47.54	A
	MOTA	1371		VAL			•	51.497	32.842	15.109	1.00 48.50	A
	MOTA	1372	С	VAL				49.150	30.342	13.389	1.00 44.12	A
_	ATOM	1373	0	VAL				48.956	30.765	12.247	1.00 44.46 1.00 40.48	A A
5	MOTA	1374	N	GLY				48.348	29.467	13.985	1.00 40.48	A
	MOTA	1375	CA	GLY					28.941	13.306		A
	MOTA	13.76	C	GLY				46.101	29.960	12.964	1.00 35.39 1.00 35.92	A
	ATOM	1377	0	GLY				46.313	31.168	13.065	1.00 33.32	A
••	ATOM	1378	N	THR				44.936	29.463	12.560 12.184	1.00 30.20	A
10	MOTA	1379	CA	THR				43.813	30.312	11.829	1.00 30.20	. A
	ATOM	1380	CB	THR				42.593 42.952	29.450 28.573	10.755	1.00 32.81	A
	ATOM	1381		THR THR				41.419	30.319	11.390	1.00 28.34	A
	ATOM	1382	C	THR				43.476	31.296	13.296	1.00 27.96	A
15	ATOM	1383	0	THR				43.212	30.907	14.434	1.00 25.46	A
13	ATOM	1384 1385	Ŋ	ALA				43.486	32.576	12.938	1.00 25.22	A
	ATOM ATOM	1386	CA	ALA				43.247	33.675	13.867	1.00 23.27	A
•	ATOM	1387	CB	ALA				42.956	34.955	13.082	1.00 22.94	A
	ATOM	1388	C			246		42.178	33.475	14.934	1.00 21.27	A
20	ATOM	1389	0	ALA				42.431	33.705	16.114	1.00 20.93	A
20	ATOM	1390	N			247		40.988	33.047	14.536	1.00 19.67	A
	ATOM	1391	CA			247		39.911	32.886	15.504	1.00 20.17	A
	ATOM	1392	CB	GLN		247		38.608	32.535	14.779	0.50 21.89	AC1
	ATOM	1393	CG	GLN		247		38.522	33.076	13.355	0.50 26.18	AC1
25	ATOM	1394	CD	GLN		247	٠.	37.220	33.794	13.064	0.50 27.30	AC1
	ATOM	1395		GLN		247		36.172	33.447	13.605	0.50 30.13	AC1
	ATOM	1396	NE2			247		37.278	34.792	12.189	0.50 28.70	AC1
	MOTA	1397	С	GLN	Α	247		40.181	31.849	16.595	1.00 19.43	A
	MOTA	1398	0	GLN	A	247		39.546	31.883	17.648	1.00 18.93	A
30	ATOM	1399	N	TYR	Α	248		41.132	30.948	16.359	1.00 18.60	A
	MOTA	1400	CA	TYR	Α	248		41.441	29.896	17.329	1.00 19.20	A
	MOTA	1401	CB	TYR	A	248		41.333	28.529	16.642	1.00 17.53	A.
	ATOM	1402	CG			248		40.013	28.362	15.927	1.00 19.32	A
	MOTA	1403	CD1	TYR	Α	248		38.859	28.010	16.625	1.00 17.69	A
35	MOTA	1404		TYR			•	37.617	27.976	15.990	1.00 18.18	A
	MOTA	1405	CD2			248		39.897	28.664	14.569	1.00 16.87	A
	MOTA	1406	CE2			248		38.665	28.635	13.924	1.00 19.17	A N
	MOTA	1407	CZ			248		37.527	28.295	14.643	1.00 19.46 1.00 18.98	A A
	MOTA	1408	OH			248		36.299	28.311	14.023 17.993	1.00 18.38	. A
40	ATOM	1409	C			248	·	42.810	30.039	18.792	1.00 20.42	A
	ATOM	1410	0			248		43.208	29.191 31.114	17.673	1.00 20.20	A
	ATOM	1411	N			249		44.841	31.343	18.251	1.00 20.91	A
	ATOM	1412	CA CB			249 249		45.542	32.532	17.570	1.00 21.18	A
15	ATOM	1413		VAL				46.821	32.896	18.317	1.00 22.45	A
45	ATOM	1414 1415		VAL				45.862	32.170	16.139	1.00 24.01	A
	ATOM ATOM	1415	C			249		44.764	31.606	19.750	1.00 21.52	A
	ATOM	1417	0	•		249		43.915	32.368	20.216	1.00 22.72	A
	ATOM	1418	N.			250		45.654	30.965	20.503	1.00 20.70	A
50	ATOM	1419	CA			250		45.697	31.133	21.951	1.00 21.65	A
50	MOTA	1420	CB			250		46.370	29.919	22.613	1.00 22.02	A
	MOTA	1421	OG			250		47.692	29.725	22.132	1.00 22.12	A
	MOTA	1422	C			250		46.476	32.402	22.280	1.00 22.13	A
	MOTA	1423	ō			250		47.332	32.828	21.511	1.00 22.77	A
55	ATOM	1424	N			251		46.180	33.029	23.425	1.00 22.23	Α
	ATOM	1425	CD			251		45.163	32.684	24.433	1.00 22.97	A
	ATOM	1426	CA			251		46.893	34.254	23.800	1.00 22.52	A
	ATOM	1427	CB	PRC) A	251		46.233	34.650	25.127	1.00 23.06	A
	ATOM	1428	CG	PRO) A	251		45.726	33.329	25.676	1.00 22.55	A

	ATOM	1429	С	PRO	A	251	4	8.414		34.115	23.907		22.15	A
	MOTA	1430	0	PRO	A	251	4	9.143		35.047	23.563		22.62	A
	MOTA	1431	N	GLU	Α	252	4	8.901	. :	32.966	24.367		20.69	A
•	MOTA	1432	CA	GLU	A.	252	5	0.347		32.772	24.500		21.40	A
5	MOTA	1433	CB	GLU	A	252	5	0.673		31.382	25.071		20.59	A
	MOTA	1434	CG	GLU	Α	252	4	9.993		30.232	24.352		21.91	A
	MOTA	1435	CD	GLU	A	252	4	8.691		29.822	25.014		21.51	A
	ATOM	1436	OE1	GLU	A	252	4	7.989		30.707	25.550		21.46	A
	MOTA	1437	OE2	\mathtt{GLU}	Α	252	4	8.367		28.613	24.993		20.23	A
10	ATOM	1438	С	GLU	A	252	5	1.071		32.970	23.167		22.99	A
	MOTA	1439	0	GLU	Α	252	5	2.191		33.480	23.136		23.17	A
	MOTA	1440	N	LEU	Α	253	5	0.441		32.576	22.064		23.00	A
	MOTA	1441	CA	LEU	Α	253	5	1.068		32.753	20.758		25.62	A
	MOTA	1442	CB	LEU	Α	253		0.277		32.029	19.669		26.75	A
15	MOTA	1443	CG	LEU	Α	253		0.743		30.620	19.296		31.87	A
	MOTA	1444		LEU				0.433		29.651	20.422		31.81	A·
	MOTA	1445	CD2	LEU				0.044		30.179	18.015		31.86	A
	MOTA	1446	С	LEU				1.201		34.228	20.371		26.94	A
	MOTA	1447	0	LEU	Α	253		2.107		34.601	19.626		27.09	A
20	MOTA	1448	N	LEU				0.297		35.059	20.877		25.83	A
	ATOM	1449	CA	LEU				0.297		36.485	20.564		27.26	A
	ATOM	1450	CB	LEU	Α	254	4	8.858		37.006	20.564		25.84	A
	MOTA	1451	CG			254	_	7.882		36.290	19.621		24.69	A
	MOTA	1452		LEU				6.459		36.724	19.932		23.64	A
25	MOTA	1453	CD2	LEU	Α	254		18.236		36.597	18.177		24.24	A
	MOTA	1454	С	LEU				51.134		37.314	21.537		30.62	A
	MOTA	1455	0	LEU	Α	254		51.633		38.383	21.187		32.35	A
	ATOM	1456	N	THR	Α	255		1.292		36.821	22.758		32.47	A
	MOTA	1457	CA	THR	Α	255		2.056		37.547	23.759		36.70	A
30	MOTA	1458	CB	THR	A	255		51.368		37.478	25.127		34.51	A
	MOTA	1459	OG1	THR				51.188		36.106	25.494		35.49	A
	MOTA	1460	CG2			255		50.013		38.166	25.077		33.40	A
	MOTA	1461	C			255		53.477		37.035	23.910		40.09	A.
	MOTA	1462	0			255		54.430		37.793	23.772		43.69	A
35	MOTA	1463	N			256		53.617		35.747	24.189		44.77	A
	MOTA	1464	CA			256		54.932		35.144	24.382		49.15	A
	MOTA	1465	CB			256		54.866		34.143	25.534		51.24	A
	MOTA	1466	CG			256		54.514		34.786	26.862		56.03	A A
	MOTA	1467	CD			256		54.053		33.780	27.893		58.83	A A
40	MOTA	1468		L GLU				54.766		32.776	28.107		62.13	A
	ATOM	1469		GLU				52.979		33.996	28.494		60.34	A
	ATOM	1470	C			256		55.475		34.456	23.137		50.09	A
	MOTA	1471	0			256		56.616		33.995	23.127			A
	MOTA	1472	N			257		54.658		34.389	22.090		51.21 51.22	A
45	ATOM	1473	•			257		55.064		33.746	20.845		0 53.28	A
	MOTA	1474	CB			257		56.244		34.502	20.227		0 55.19	A
	ATOM	1475	CG			257		56.558		34.125	18.790		0 57.52	A
	ATOM	1476	CD			257		57.709		34.961	18.253		0 58.52	A
	ATOM	1477	CE			257		57.952		34.694	16.777		0 60.88	A
50	MOTA	1478	NZ			257		58.29		33.268	16.515		0 50.74	A
	ATOM	1479	C			257		55.46'		32.302	21.138 20.577		0 50.74	A
	ATOM	1480	0			257		56.431		31.790 31.654	20.577		0 48.07	A
	MOTA	1481	N			258		54.72		30.273	22.027		0 46.87	A
	MOTA	1482	CA			258		54.99:		30.273			0 48.88	A
55	MOTA	1483	CB			258		55.59		30.229			0 53.14	A
	MOTA	1484				258		54.74		29.415			0 44.07	A
	MOTA	1485	C			258		53.73					0 44.17	A
	MOTA	1486	0			258		52.61		29.932			0 38.30	A
	ATOM	1487	N	ALA	. P	259		53.91	. 7	28.105	22.204	. 1.0	, ,,,,,	

	ATOM	1488	CA	ALA A	259	52.793	27.180	22.127	1.00 34.73	· A
	ATOM	1489	CB	ALA A	259	52.551	26.779	20.684	1.00 34.16	A
	ATOM	1490	C	ALA A	259	53.042	25.940	22.977	1.00 32.34	Α
	ATOM	1491	0	ALA A	259	54.172	25.459	23.086	1.00 31.81	A
5	ATOM	1492	N	CYS A	260	51.975	25.428	23.579	1.00 28.58	A
	ATOM	1493	CA	CYS A	260	52.056	24.244	24.425	1.00 26.27	A
	ATOM	1494	CB	CYS A	260	52.183	24.654	25.892	1.00 26.53	A
	ATOM	1495	SG	CYS A	260	50.846	25.739	26.469	1.00 32.91	A
	MOTA	1496	C	CYS A	260	50.786	23.435	24.224	1.00 22.83	A
10	MOTA	1497	0	CYS A	260	49.892	23.856	23.495	1.00 22.14	A
	MOTA	1498	N	LYS A	261	50.706	22.277	24.868	1.00 20.02	A
	MOTA	1499	CA	LYS A	261	49.526	21.434	24.744	1.00 20.65	A
	ATOM	1500	CB	LYS A	261	49.619	20.243	25.696	1.00 23.28	A
	ATOM	1501	CG	LYS A	261	50.716	19.253	25.347	1.00 27.44	A
15	ATOM	1502	CD	LYS A	261	50.732	18.117	26.350	1.00 29.98	A
	MOTA	1503	CE	LYS A	261	51.922	17.203	26.134	1.00 32.34	A
	MOTA	1504	NZ	LYS A	261	51.940	16.121	27.153	1.00 33.28	A
	MOTA	1505	C	LYS A	261	48.268	22.229	25.062	1.00 19.20	A
	ATOM	1506	0	LYS A	261	47.253	22.092	24.387	1.00 18.08	A
20	ATOM	1507	N	SER A	262	48.358	23.068	26.089	1.00 16.92	Α
	ATOM	1508	CA	SER A	262	47.235	23.883	26.534	1.00 18.13	A
	ATOM	1509	CB	SER A	262	47.644	24.698	27.770	1.00 18.27	A
	ATOM	1510	OG	SER A	262	46.517	25.258	28.421	1.00 22.53	A
	ATOM	1511	С	SER A	262	46.736	24.811	25.424	1.00 16.77	A
25	ATOM	1512	0	SER A	262	45.591	25.254	25.450	1.00 15.69	A
	MOTA	1513	N	SER A	263	47.595	25.118	24.456	1.00 16.44	Α
	MOTA	1514	CA	SER A	263	47.175	25.970	23.347	1.00 16.89	A
	MOTA	1515	CB	SER A	263	48.340	26.228	22.382	1.00 18.49	A
	MOTA	1516	OG	SER A	263	49.402	26.909	23.031	1.00 22.10	A
30	MOTA	1517	C	SER A	263	46.040	25.257	22.612	1.00 17.79	A
	MOTA	1518	0	SER A	263	45.099	25.898	22.148	1.00 17.57	A
	MOTA	1519	N	ASP A	264	46.119	23.928	22.517	1.00 16.30	Α.
	MOTA	1520	CA	ASP A	264	45.069	23.166	21.836	1.00 16.72	A
	MOTA	1521	CB	ASP A	264	45.483	21.704	21.620	1.00 15.92	Α
35	MOTA	1522	CG	ASP A	264	46.544	21.539	20.548	1.00 17.93	A
	MOTA	1523	OD1	ASP A	264	46.642	22.412	19.661	1.00 16.78	A
	MOTA	1524	OD2	ASP A	264	47.265	20.515	20.579	1.00 16.64	A
	ATOM	1525	C	ASP A	264	43.773	23.194	22.646	1.00 17.67	A
	ATOM	1526	0	ASP A	264	42.681	23.197	22076	1.00 18.27	A
40	ATOM	1527	N	LEU A	265	43.898	23.205	23.974	1.00 15.49	A
	ATOM	1528	CA	LEU A		42.730	23.232	24.849	1.00 14.75	. A
	ATOM	1529	CB	LEU A	265	43.147	23.038	26.313	1.00 11.38	A
	ATOM	1530	CG	LEU A	265	43.711	21.641	26.621	1.00 14.04	A
	MOTA	1531	CD1	LEU A	265	44.249	21.579	28.052	1.00 13.96	A
45	MOTA	1532	CD2	LEU A	265	42.619	20.603	26.416	1.00 11.62	A
	ATOM	1533	C	LEU A		41.999	24.557	24.675	1.00 15.13	A
	MOTA	1534	0	LEU A	265	40.777	24.620	24.785	1.00 16.75	A
	MOTA	1535	N	TRP A	266	42.746	25.622	24.405	1.00 16.08	A
	MOTA	1536	CA	TRP A	266	42.118	26.918	24.184	1.00 16.96	A
50	MOTA	1537	CB	TRP A	-	43.176	28.015	24.023	1.00 17.28	A
	MOTA	1538	CG	TRP A		42.618	29.326	23.521	1.00 20.54	A
	MOTA	1539	CD2	TRP A	266	42.313	30.490	24.301	1.00 20.07	, A
	MOTA	1540	CE2	TRP A	266	41.782	31.459	23.417	1.00 20.46	A
	MOTA	1541		TRP A		42.435	30.810	25.660	1.00 20.68	A
55	MOTA	1542		TRP A		42.270	29.631	22.231	1.00 19.53	A
	ATOM	1543		TRP A		41.769	30.908	22.163	1.00 19.61	A
	MOTA	1544		TRP A		41.372	32.727	23.850	1.00 20.90	A
	MOTA	1545		TRP A		42.026	32.073	26.091	1.00 19.45	A
	MOTA	1546	CH2	TRP A	266	41.501	33.015	25.185	1.00 20.71	A

				,												
	ATOM	1547	С	TRP	Α	266	41	284	26.795	5 22	2.913		0 17.2		A	
	ATOM	1548	0	TRP	Α	.266	40	.139	27.240		2.863		0 18.0		A	
	ATOM	1549	N	ALA	Α	267	41	. 863	26.181	1 2	1.886		0 17.		A	
	MOTA	1550	CA	ALA	Α	267	41	. 155	25.990	0 20	0.626		0 16.3		A	
5	ATOM	1551	CB	ALA	A	267	42	.050	25.290		9.621		0 14.2		A	
	MOTA	1552	C	ALA	Α	267	39	.901	25.159		0.891		0 16.2		A	
	ATOM	1553	0	ALA	Α	267	38	.835	25:436	_	0.346		0 16.4		A	
	MOTA	1554	N	LEU	A	268	40	.031	24.144		1.739		0 16.		A	
	MOTA	1555	CA	PE O	A	268	38	.890	23.299	9 22	2.084		0 17.		A	
10	MOTA	1556	CB	LEU	A	268	39	.292	22.260		3.139		0 15.		A	
	MOTA	1557	CG	LEU				.158	21.429		3.754		0 19.		A	
	ATOM	1558	CD1	LEU	Α	268	37	.505	20.578		2.678		0 16.		A	
	ATOM	1559	CD2	LEU	Α	268	38	.718	20.53		4.881		0 17.		A	
	ATOM	1560	C	LEU				.766	24.17		2.628		0 15.		A	
15	ATOM	1561	0	LEU				.603	24.03		2.247		0 15.		A	
	MOTA	1562	N	GLY				.119	25.09		3.520		0 14.		A	
	MOTA	1563	CA	GLY	A	269		.124	25.989		4.092		0 13.		A	
	MOTA	1564	С	GLY				.406	26.80		3.031		0 14.			
	MOTA	1565	0	GLY				.193	27.01		3.114		0 14.		<i>P</i> .	
20	ATOM	1566	N	CYS				.146	27.27		2.030		0 13.		. A	
	MOTA	1567	CA	CYS				.539	28.06		0.958		0 16.		7	
	MOTA	1568	CB	CYS				.611	28.63		0.023		0 15.		7	
	MOTA	1569	SG	CYS				.751	29.81	-	0.780		0 20.			<i>,</i>
	MOTA	1570	C	CYS				.598	27.17		0.140		0 17.			<i>}</i> 7
25	MOTA	1571	0	CYS				.516	27.60		9.741		0 18.			4
	MOTA	1572	N	ILE				.022	25.93		9.887		0 16.			
	MOTA	1573	CA			271		.221	25.00		9.104		0 16.		7	4
	ATOM	1574	CB			271		.038	23.74		8.778		0 16.			A.
	ATOM	1575	-	ILE				.155	22.69		8.102		0 16.			A.
30	MOTA	1576		ILE				.222	24.12		7.882		0 15. 0 14.			A.
	MOTA	1577		ILE				.239	23.01		7.690		0 14.			A.
	MOTA	1578	C			271		.920	24.62		9.809		0 17.			A.
	MOTA	1579	0			271		.865	24.57		9.179		0 16.			A.
	MOTA	1580	N			272		.990	24.35		1.111 1.862		0 18.			A
35	MOTA	1581	CA			272		.785	24.02		3.346		0 17.			A
	ATOM	1582	CB			272		.097	23.74		4.152		0 17.			A
	ATOM	1583		ILE				.796	23.66 22.43		3.481		0 19.			A
	ATOM	1584		ILE				.877	22.43		4.886		0 18.			A.
40	ATOM	1585		ILE		272		.446	25.20		1.776		0 19.			A
40	ATOM	1586	C					.624	25.20		1.554		0 20.			A
	ATOM	1587	0			272 273		.362	26.40		1.947		0 18.			A
	MOTA MOTA	1588 1589	N CA			273		.553	27.61		1.881		0 20.			A
	ATOM	1590	CB			273		.418	28.84		2.162		0 18.		1	A
45			CG			273		.663	30.16		2.125		0 20.		1	A
45	MOTA MOTA	1591 1592		TYR				.229	30.70	9 2	0.916	1.0	0 20.			Α
	ATOM	1593		TYR				.536	31.91		0.880		0 20.			A
	ATOM	1594		TYR				.383	30.85		3.302		0 19.			A
	ATOM	1595	CE2			273		.691	32.06		3.280		0 20.			A
50	ATOM	1596	CZ			273		.271	32.58		2.067		0 21.			Α
50	ATOM	1597	OH			273		.588	33.77		2.049		0 21.	86		A
	ATOM	1598	C			273		.902	27.73		0.507		0 21.			Α
	ATOM	1599	ō			273		.719	28.04		0.401		00 22.			Α.
	ATOM	1600	N			274		.676	27.45		9.461		0 21.	05		Α
55	ATOM	1601	CA			274		.176	27.53		8.095		00 21.			Α
55	MOTA	1602	CB			274		.323	27.34		17.097	1.0	00 21			A
•	ATOM	1603	CG			274		934	27.59		15.645	1.0	00 23			A
	ATOM	1604	CD			274		.131	27.58		L4.706		00 24			A
	ATOM	1605		LGLN				.276	27.44	16]	15.139	1.0	00 22	.51		A

	ATOM	1606	NE2	GLN	Α	274	32	.870	27.750	13.413	1.00	22.96	A
	ATOM	1607	С	GLN	Α	274	30	.076	26.517	17.828		21.51	A
	ATOM	1608	0	GLN	A	274	29	.123	26.806	17.108	1.00	20.50	A
	ATOM	1609	N	LEU	A	275	30	.207	25.324	18.403	1.00	21.44	A
5	ATOM	1610	CA	LEU	A	275	29	.196	24.282	18.208		20.95	A
•	MOTA	1611	CB	LEU	A	275	29	.645	22.958	18.846		19.11	A
	ATOM	1612	CG	LEU	Α	275	30	.775	22.182	18.159		21.43	A
	ATOM	1613	CD1	LEU	Α	275	31	.118	20.936	18.963	1.00	17.64	A
	MOTA	1614	CD2	LEU	A	275	30	.342	21.795	16.754	1.00	20.34	A
10	MOTA	1615	C	LEU	A	275	27	.860	24.697	18.815		21.32	A
	MOTA	1616	0	LEU	Α	275	26	.802	24.461	18.229		19.75	Α
	ATOM	1617	N	VAL	Α	276	27	.921	25.322	19.987		19.10	A
	MOTA	1618	CA	$_{ m LAV}$	Α	276	26	.724	25.750	20.702		22.47	A
	ATOM	1619	CB	VAL	A	276	27	.011	25.882	22.217		20.87	A
15	ATOM	1620	CG1	VAL	A	276	25	.742	26.291	22.957		19.68	A
	MOTA	1621	CG2	VAL	A	276		.550	24.558	22.766		19.43	A
	MOTA	1622	С	VAL	A	276	26	.127	27.075	20.211		23.89	A
	MOTA	1623	0	VAL	Α	276	24	.910	27.199	20.070		24.90	A
	MOTA	1624	И	ALA	А	277	26	.983	28.062	19.965		24.56	A
20	MOTA	1625	CA	ALA	Α	277	26	5.533	29.374	19.518		24.72	A
	ATOM	1626	CB	ALA	A	277	27	7.504	30.444	19.999		24.36	A
	MOTA	1627	C	ALA	A	277	26	5.378	29.458	18.005		25.76	A
	MOTA	1628	0	ALA	A	277	25	5.577	30.242	17.502		26.39	A
	MOTA	1629	N	GLY	A	278	27	7.142	28.651	17.280		25.13	A
25	MOTA	1630	CA	GLY	Α	278	27	7.062	28.673	15.834		25.58	· A
	ATOM	1631	C	GLY	Α	278	28	3.163	29.524	15.231		26.50	A
	MOTA	1632	0	GLY	Α	278	28	3.374	29.510	14.015		28.17	A
	ATOM	1633	N	LEU	Α	279	28	3.866	30.262	16.086		24.44	A
•	MOTA	1634	CA	LEU	Α	279	29	9.962	31.130	15.656		25.21	A
30	ATOM	1635	CB	LEU	A	279	29	9.468	32.575	15.500		25.78	A
	ATOM	1636	CG	LEU	A	279	28	3.364	32.899	14.490		28.17	. A
	MOTA	1637	CD1	LEU	A	279	27	7.922	34.344	14.684		26.60	A
	MOTA	1638	CD2	LEU	A	279	28	3.862	32.670	13.071		26.52	A
	MOTA	1639	C	LEU	A	279		1.093	31.116	16.687		23.47	A
35	ATOM	1640	0	LEU	A	279		0.848	30.994	17.882		24.44	A
	MOTA	1641	N	PRO	A	280		2.349	31.239	16.236		23.35	A
	ATOM	1642	CD			280		2.831	31.404	14.855		22.26	A
	MOTA	1643	CA			280		3.464	31.239	17.189		23.81	A
	MOTA	1644	CB			280		4.692	31.293	16.282		23.24	A
40	MOTA	1645	CG			280		4.189	32.020	15.073		24.89	A
	MOTA	1646	С			280		3.353	32.444	18.137		22.69	A A
	ATOM	1647	0			280		2.750	33.457	17.788		22.11	A
	MOTA	1648	N			281		3.939	32.344	19.345			A
	ATOM	1649	CD			281		4.810	31.223	19.734		21.37	A
45	MOTA	1650	CA			281		3.935	33.375	20.395		23.67	A
	MOTA	1651	CB			281		4.781	32.751	21.509		25.24	A
	ATOM	1652	CG			281		4.749	31.287	21.219		23.75	A
	ATOM	1653	. C			281		4.481	34.752	20.017		23.75	Ā
	ATOM	1654	0			281		3.869	35.781	20.317		22.17	A
50	ATOM	1655	N			282		5.644	34.763	19.379		23.16	A
	ATOM '		CA			282		6.293	36.007	18.998 19.406		21.01	A
	ATOM	1657	CB			282		7.765	35.943			22.66	A
	ATOM	1658	CG			282		7.975	35.482 36.361	20.822		20.06	A
	ATOM	1659		PHE				7.806	34.151	21.888		20.72	A
55	ATOM	1660		PHE				8.291	35.921	23.206		22.66	A
	ATOM	1661	-	PHE				7.947		23.206		20.97	A
	MOTA	1662		PHE				8.433		23.466		19.58	A
	ATOM	1663	cz			282		8.261	36.263	17.503		24.39	A
	ATOM	1664	С	PHE	Ρ	. 282	3	6.169	30.203	11.503	1.00		

	ATOM	1665	0	PHE A	282	36.802	35.585	16.694	1.00 25.80	A
	ATOM	1666	N	ARG A	283	35.355	37.248	17.142	1.00 24.99	A
	ATOM	1667	CA	ARG A		35.141	37.594	15.741	1.00 26.33	A
	MOTA	1668	CB	ARG A	283	33.721	37.209	15.316	1.00 28.91	A
5	ATOM	1669	CG	ARG A		33.293	35.808	15.724	1.00 30.27	A
_	ATOM	1670	CD	ARG A	283	31.904	35.493	15.188	1.00 33.36	A
	ATOM	1671	NE	ARG A	283	30.890	36.392	15.733	1.00 32.76	A
	ATOM	1672	CZ	ARG A		30.372	36.287	16.952	1.00 34.79	A
	ATOM	1673		ARG A		30.767	35.317	17.768	1.00 35.77	A
10	ATOM	1674		ARG A		29.458	37.156	17.359	1.00 36.12	A
10	ATOM	1675	C	ARG A		35.328	39.096	15.544	1.00 26.47	A
	ATOM	1676	ō	ARG A		35.029	39.888	16.438	1.00 26.28	Α
	ATOM	1677	N	ALA A		35.818	39.486	14.373	1.00 26.70	A
		1678	CA	ALA A		36.033	40.899	14.079	1.00 27.84	A
15	ATOM		CB	ALA A		37.188	41.442	14.914	1.00 26.24	Α
15	ATOM	1679		ALA A		36.327	41.077	12.602	1.00 28.35	A
•	ATOM	1680	C			36.560	40.101	11.891	1.00 29.91	A
	ATOM	1681	0	ALA A		36.332	42.329	12.153	1.00 29.29	A ·
	ATOM	1682	N	GLY A		36.577	42.631	10.753	1.00 29.52	A
00	MOTA	1683	CA	GLY A		37.893	42.156	10.168	1.00 30.12	A
20	ATOM	1684	C	GLY A			41.862	8.976	1.00 30.60	A
	ATOM	1685	0	GLY A		37.974		10.983	1.00 30.00	A
	ATOM	1686	N	ASN A		38.939	42.097	10.489	1.00 26.45	A
	MOTA	1687	CA	ASN A		40.231	41.644	9.945		A
	MOTA	1688	CB	ASN A		41.050	42.825		1.00 26.11 1.00 27.83	A
25	MOTA	1689	CG	ASN A		41.310	43.900	10.990		A
	MOTA	1690		ASN A		41.877	43.631	12.049	1.00 27.84	A
	MOTA	1691	. ND2			40.908	45.131	10.685	1.00 25.95	A
	MOTA	1692	С	ASN A		40.997	40.924	11.584	1.00 26.03	
	MOTA	1693	0	ASN A		40.540	40.851	12.723	1.00 25.66	A
30	MOTA	1694	N	GLU I		42.162	40.391	11.239	1.00 24.81	A
	MOTA	1695	CA	GLU A		42.965	39.662	12.206	1.00 27.59	A
	MOTA	1696	CB	GLU A		44.145	38.985	11.510	1.00 30.17	A
	ATOM	1697	CG	GLU A		43.776	37.632	10.931	1.00 38.21	A
	MOTA	1698	CD		A 287	44.900	36.998	10.140	1.00 41.86	A
35	ATOM	1699		GLU A		46.061	37.036	10.608	1.00 43.08	A
	MOTA	1700	OE2	GLU A		44.612	36.449	9.052	1.00 45.22	A
	MOTA	1701	С		A 287	43.459	40.485	13.383	1.00 25.05	A
	ATOM	1702	0		A 287	43.382	40.030	14.521	1.00 26.41	A
	MOTA	1703	N		882	43.966	41.685	13.122	1.00 23.04	A
40	MOTA	1704	CA		A 288	44.460	42.528	14.205	1.00 22.34	A
	MOTA	1705	CB		A 288	44.867	43.913	13.691	1.00 21.07	A
	ATOM	1706	CG		A 288	45.275	44.858	14.805	1.00 21.07	A
	ATOM	1707	CD1		A 288	46.533	44.762	15.405	1.00 21.23	A
	MOTA ·	1708	. CE1	TYR	A 288	46.891	45.588	16.475	1.00 20.43	A
45	ATOM	1709	CD2	TYR		44.380	45.809	15.302	1.00 22.32	A.
	ATOM	1710	CE2		A 288	44.725	46.637	16.373	1.00 23.28	A
	ATOM	1711	CZ	TYR Z	A 288	45.981	46.518	16.953	1.00 22.96	Α
	MOTA	1712	OH		A 288	46.316	47,313	18.024	1.00 23.18	A
	ATOM	1713	C	TYR .	A 288	43.402	42.698	15.288	1.00 21.38	·Α
50	ATOM	1714	0		A 288	43.710	42.616	16.473	1.00 22.09	A
	MOTA	1715	N	LEU .	A 289	42.159	42.939	14.874	1.00 21.88	A
•	MOTA	1716	CA		A 289	41.055	43.130	15.811	1.00 21.98	A
	MOTA	1717	CB		A 289	39.821	43.673	15.078	1.00 22.90	A
	MOTA	1718	CG		A 289	39.896	45.130	14.601	1.00 26.52	A
55	MOTA	1719		LEU .		38.706	45.436	13.696	1.00 26.55	A
	MOTA	1720	CD2	LEU		39.914	46.071	15.807	1.00 23.13	A
	MOTA	1721	C	LEU	A 289	40.686	41.849	16.560	1.00 21.24	A
	MOTA	1722	0		A 289	40.256	41.897	17.715	1.00 20.72	A
	MOTA	1723	N	ILE	A 290	40.843	40.708	15.900	1.00 19.62	A

	ATOM	1724	CA	ILE A	290	40	.538	39.433	16.533		18.54	A
	ATOM	1725	CB	ILE A	290	40	.560	38.281	15.509		18.52	A
	MOTA	1726	CG2	ILE A	290	40	.503	36.934	16.234		17.63	A
	MOTA	1727	CG1	ILE A	290	39	.378	38.429	14.545		18.88	A
5	ATOM	1728	CD1	ILE A		39	.421	37.483	13.357		19.81	A
	ATOM	1729	С	ILE A	290		.578	39.167	17.618		19.09	A
	ATOM	1730	0	ILE A	290	41	.236	38.788	18.737		18.20	A
	ATOM	1731	N	PHE A	291		.849	39.376	17.286		18.76	A
	MOTA	1732	CA	PHE A			.925	39.156	18.247		20.75	A
10	MOTA	1733	CB	PHE A			.286	39.434	17.606		20.71	A
	MOTA	1734	CG	PHE A			.644	38.480	16.503		22.92	A A
	MOTA	1735		PHE A			.065	37.214	16.443		22.98 22.91	A
	MOTA	1736	-	PHE A			.588	38.830	15.543			A
	MOTA	1737		PHE A			.423	36.310	15.440		24.51 25.54	A
15	MOTA	1738		PHE A			.954	37.931	14.535		23.29	A
	MOTA	1739	CZ	PHE A			.370	36.670	14.485		21.72	A
	MOTA	1740	С	PHE A			.739	40.061	19.451 20.593		22.32	A
	ATOM	1741	0	PHE A			.992	39.671	19.178		23.27	A
	MOTA	1742	N	GLN A			.284	41.275	20.216		24.01	A
20	ATOM	1743	CA	GLN A			.055	42.264 43.559	19.562		25.77	A
	ATOM	1744	CB	GLN A			:.574 :.577	44.773	20.447		28.45	A
	ATOM	1745	CG	GLN A			.469	46.057	19.638		29.83	A
	MOTA	1746	CD	GLN A GLN A			520	46.244	18.872		27.16	A
25	MOTA	1747					.449	46.944	19.799		27.61	A
25	MOTA	1748	NE2 C	GLN A			2.018	41.733	21.204		22.97	Α
	MOTA	1749 1750	0	GLN A			2.200	41.832	22,415		21.64	Α
	MOTA	1751	И	LYS A).937	41.154	20.687		21.82	A
	ATOM ATOM	1751	CA	LYS A			895	40.612	21.558		22.18	A
30	ATOM	1753	CB	LYS A			3.664	40.223	20.740	1.00	22.69	Α
50	ATOM	1754	CG	LYS A			7.919	41.407	20.153	1.00	25.78	A
	ATOM	1755	CD	LYS A			5.651	40.961	19.429	1.00	27.88	A
	ATOM	1756	CE	LYS A		35	5.857	42.161	18.926	1.00	30.85	A
	ATOM	1757	NZ	LYS A		34	1.612	41.750	18.214	1.00	32.98	~ A
35	ATOM	1758	C	LYS A	293	40	398	39.398	22.343		21.20	A
	MOTA	1759	0	LYS A	293	40	0.041	39.204	23.509		22.01	A
	MOTA	1760	N	ILE A	294	43	1.226	38.583	21.702		19.91	Α
	MOTA	1761	CA	ILE A	294	41	1.774	37.394	22.347		20.28	A
	ATOM	1762	CB	ILE A	294	42	2.631	36.575	21.349		18.98	A
40	MOTA	1763		ILE A		43	3.481	35.550	22.098		17.70	A
	ATOM	1764		ILE A		4:	1.716	35.897	20.318		17.93	A
	MOTA	1765	CD1	ILE A			2.467	35.237	19.178		16.21	A
	ATOM	1766	C	ILE A			2.618	37.727	23.587		21.94	A A
	MOTA	1767	0	ILE A			2.366	37.199	24.673		20.86	_
45	MOTA	1768	N	ILE A			3.610	38.600	23.439		21.88	A A
	MOTA	1769	CA	ILE A			4.461	38.934	24.582		24.25	A
	ATOM	1770	CB	ILE A			5.668		24.175		24.61	A
	ATOM	1771		ILE A			6.514	39.066	23.140		24.51	A
	MOTA	1772		ILE A			5.189	41.151	23.637		26.69	A
50	MOTA	1773		L ILE A			6.317	42.149 39.636	.23.433 25.717		24.80	A
•	MOTA	1774	C	ILE A			3.720 4.214	39.687	26.842		24.76	A
	ATOM	1775	0	ILE A				40.173	25.425		25.33	A
	MOTA	1776	N	LYS A	1 296		2.539 1.743	40.173	26.444		26.80	, A
	MOTA	1777	CA		A 296		1.178	42.170	25.894		0 27.39	A
55	MOTA	1778	CB CG		A 296		2.240	43.141	25.413		0 31.79	A
	ATOM	1779 1780	CD		A 296		1.634	44.410	24.826		0 35.56	A
	ATOM	1780	CE		A 296		1.009	45.283	25.900		0 39.29	A
	ATOM ATOM	1782	NZ		A 296		0.564	46.603	25.357		0 41.72	A
	ATOM	1102	114	210 1		•						

	ATOM	1783	С	LYS A	296	40.593	39.958	26.893	1.00 25.50	A
	ATOM	1784	0	LYS A		39.770	40.361	27.713	1.00 24.02	A
	ATOM	1785	N	LEU A		40.550	38.742	26.349	1.00 25.67	A
	ATOM	1786	CA	LEU A	297	39.500	37.777	26.666	1.00 25.16	Α
5	MOTA	1787	СВ	LEU A		39.632	37.285	28.111	1.00 24.80	A
-	ATOM	1788	CG	LEU A		38.766	36.068	28.460	1.00 26.43	A
	ATOM	1789	CD1	LEU A	297	39.238	34.852	27.646	1.00 26.70	A
	MOTA	1790	CD2	LEU A	297	38.856	35.777	29.951	1.00 24.84	A
	ATOM	1791	C	LEU A	297	38.151	38.459	26.467	1.00 25.11	A
10	ATOM	1792	0	LEU A	297	37.261	38.378	27.309	1.00 25.28	A
	ATOM	1793	N	GLU A	298	38.007	39.127	25.331	1.00 24.98	A
	ATOM	1794	CA	GLU A	298	36.786	39.847	25.023	1.00 25.31	A
	ATOM	1795	СВ	GLU A	298	37.143	41.139	24.291	1.00 27.13	A
	ATOM	1796	ĊĠ	GLU A	298	35.991	42.092	24.108	1.00 31.28	. A
15	ATOM	1797	CD	GLU A		36.419	43.362	23.410	1.00 34.40	A
• •	ATOM	1798		GLU A		37.348	44.027	23.918	1.00 35.90	A
	ATOM	1799		GLU A		35.832	43.693	22.359	1.00 36.16	A
	ATOM	1800	C	GLU A		35.766	39.057	24.207	1.00 23.79	A
	ATOM	1801	ō	GLU A		35.832	39.017	22.979	1.00 24.35	A
20	ATOM	1802	N	TYR A		34.825	38.427	24.902	1.00 23.45	Α
20	ATOM	1803	CA	TYR A		33.760	37.663	24.265	1.00 23.98	A
	ATOM	1804	СВ	TYR A		34.264	36.304	23.755	1.00 20.13	A
	ATOM	1805	CG	TYR A		34.348	35.233	24.828	1.00 21.17	Α
	ATOM	1806		TYR A		35.336	35.279	25.810	1.00 19.32	A
25	ATOM	1807		TYR A		35.389	34.332	26.826	1.00 19.30	A
23	ATOM	1808	CD2			33.410	34.201	24.888	1.00 18.96	A
	ATOM	1809	CE2			33.456	33.243	25.907	1.00 19.41	A
	ATOM	1810	CZ	TYR A		34.449	33.321	26.870	1.00 18.79	A
	ATOM	1811	OH	TYR A		34.511	32.401	27.881	1.00 18.77	A
30	ATOM	1812	C	TYR A		32.699	37.437	25.331	1.00 25.20	A
30	ATOM	1813	ō	TYR A		32.942	37.681	26.506	1.00 26.46	A
	ATOM	1814	N	ASP A		31.522	36.981	24.927	1.00 26.94	Α
	ATOM	1815	CA	ASP A		30.467	36.710	25.891	1.00 30.60	A
	ATOM	1816	СВ	ASP A		29.665	37.981	26.179	1.00 35.86	A
35	ATOM	1817	CG	ASP A		29.228	38.687	24.923	1.00 42.04	A
33	ATOM	1818		L ASP A		28.450	38.088	24.149	1.00 45.98	A
	ATOM	1819		ASP A		29.666	39.840	24.707	1.00 45.69	A
	MOTA	1820	C	ASP A		29.564	35.608	25.363	1.00 29.26	A
	ATOM	1821	Ö	ASP A		29.590	35.299	24.172	1.00 28.64	A
40	MOTA	1822	N	PHE A		28.778	35.011	26.253	1.00 28.96	A
70	MOTA	1823	CA		301	27.884	33.924	25.871	1.00 30.48	A
	MOTA	1824	СВ		A 301	27.818	32.854	26.968	1.00 29.17	A
	MOTA	1825	CG	•	301	29.147	32.279	27.356	1.00 29.29	A
	ATOM	1826		1 PHE A		29.978	32.949	28.245	1.00 27.31	A
45	ATOM	1827		2 PHE A		29.560	31.050	26.845	1.00 27.89	A
40	ATOM	1828		1 PHE A		31.205	32.403	28.625	1.00 28.83	A
	ATOM	1829		PHE A		30.781	30.498	27.217	1.00 28.05	A
	ATOM	1830	CZ.		A 301	31.605	31.175	28.110	1.00 28.27	A
	ATOM	1831	C		A 301	26.459	34.384	25.619	1.00 32.20	A
50	ATOM	1832	o		A 301	25.946	35.261	26.317		A
20		1833	N.		A 302	25.798	33.804	24.607	1.00 33.29	A
	MOTA MOTA	1834	CD		A 302	26.313	32.943	23.529	1.00 34.04	A
		1835	CA		A 302	24.415	34.199	24.341	1.00 35.24	A
	ATOM ATOM	1836	CB		A 302	24.144	33.608	22,959	1.00 34.01	A
55	ATOM	1837	CG		A 302	25.041	32.413	22.921	1.00 35.48	A
رر	ATOM	1838	C		A 302	23.567	33.561	25.444	1.00 37.39	A
	ATOM	1839			A 302	23.935	32.518	25.986	1.00 38.49	A
		1840			A 303	22.447	34.188	25.783		A
	ATOM	1841			A 303	21.572	33.692	26.843		A
	ATOM	7047	Cr3	ישוני						

	ATOM	1842	CB	ALA	Α	303	20.280	34.506	26.862	1.00 41.66	A
	ATOM	1843	C	ALA	A	303	21.238	32.197	26.814	1.00 41.25	A
	ATOM	1844	0	ALA	A	303	21.253	31.537	27.854	1.00 43.16	A
	ATOM	1845	N	ALA	Α	304	20.945	31.665	25.631	1.00 41.04	Α
5	ATOM	1846	CA	ALA	Α	304	20.569	30.258	25.480	1.00 40.66	A
	ATOM	1847	CB	ALA	Α	304	20.121	30.004	24.040	1.00 41.36	A.
	ATOM	1848	C	ALA	Α	304	21.628	29.223	25.876	1.00 39.61	. А
	ATOM	1849	0	ALA	A	304	21.298	28.156	26.395	1.00 40.61	. A
	MOTA	1850	N	PHE	A	305	22.891	29.543	25.617	1.00 36.21	. А
10	MOTA	1851	CA	PHE	A	305	24.022	28.662	25.909	1.00 32.08	A
	ATOM	1852	CB	PHE	A	305	25.259	29.519	26.187	1.00 29.46	. A
	ATOM	1853	CG	PHE	Α	305	26.536	28.917	25.690	1.00 28.15	A
	MOTA	1854	CD1	PHE	A	305	27.146	27.875	26.377	1.00 26.20	A
	ATOM	1855	CD2	PHE	Α	305	27.127	29.386	24.521	1.00 27.05	A
15	MOTA	1856	CE1	PHE	Α	305	28.330	27.308	25.908	1.00 26.92	. A
	MOTA	1857	CE2	PHE	Α	305	28.312	28.826	24.042	1.00 26.62	. A
	ATOM	1858	CZ	PHE	Α	305	28.914	27.786	24.737	1.00 26.61	. А
	ATOM	1859	С	PHE	Α	305	23.811	27.664	27.057	1.00 30.09) . A
	ATOM	1860	0	PHE	Α	305	23.518	28.051	28.187	1.00 31.51	. А
20	ATOM	1861	N.	PHE	Α	306	23.964	26.378	26.758	1.00 27.03	. A
	ATOM	1862	CA	PHE	A	306	23.801	25.334	27.769	1.00 26.30) A
	MOTA	1863	CB	PHE	Α	306	24.157	23.970	27.170	1.00 25.03	A
	ATOM	1864	CG	PHE	Α	306	23.548	23.725	25.815	1.00 27.24	A
	MOTA	1865	CD1	PHE	Α	306	22.170	23.831	25.622	1.00 28.40) A
25	MOTA	1866	CD2	PHE	Α	306	24.350	23.386	24.728	1.00 27.84	. A
	MOTA	1867	CE1	PHE	A	306	21.601	23.603	24.365	1.00 28.05	5 A
	MOTA	1868	CE2	PHE	A	306	23.792	23.155	23.465	1.00 28.33	L A
	MOTA	1869	cz	PHE	Α	306	22.415	23.263	23.283	1.00 28.00) A
	ATOM	1870	С	PHE	A	306	24.711	25.652	28.961	1.00 26.23	A A
30	ATOM	1871	0	PHE	Α	306	25.927	25.775	28.811	1.00 25.59	A
	ATOM	1872	N	PRO	A	307	24.125	25.796	30.163	1.00 26.67	7 A
	ATOM	1873	CD	PRO	A	307	22.685	25.625	30.430	1.00 27.95	a A
	MOTA	1874	CA	PRO	Α	307	24.842	26.110	31.405	1.00 26.59) A
	ATOM	1875	CB	PRO	Α	307	23.795	25.832	32.481	1.00 26.14	ł A
35	MOTA	1876	CG	PRO	Α	307	22.531	26.250	31.803	1.00 27.86	5 A
	MOTA	1877	С	PRO	Α	307	26.145	25.355	31.659	1.00 25.58	3 · A
	MOTA	1878	0	PRO	A	307	27.189	25.964	31.900	1.00 22.65	5 A
	MOTA	1879	N	LYS	Α	308	26.085	24.031	31.620	1.00 24.46	5 A
	MOTA	1880	CA	LYS	Α	308	27.274	23.232	31.867	1.00 23.93	l A
40	MOTA	1881	CB	LYS	Α	308	26.887	21.760	32.024	1.00 23.25	5 A
	MOTA	1882	CG	LYS	Α	308	26.062	21.532	33.285	1.00 28.49	9 A
	MOTA	1883	$^{\rm CD}$	LYS	A	308	25.618	20.093	33.466	1.00 30.17	7. A
	ATOM	1884	CE	LYS	Α	308	24.760	19.973	34.722	1.00 33.1	
	MOTA	1885	NZ	LYS	Α	308	24.122	18.636		1.00 34.13	
45	ATOM	1886	C	LYS	Α	308	28.314	23.426	30.769	1.00 22.84	
	MOTA	1887	0	LYS	Α	308	29.514	23.411	31.042	1.00 22.46	
	MOTA	1888	N	ALA	A	309	27.861	23.621	29.534	1.00 21.59	
	ATOM	1889	CA	ALA	Α	309	28.792	23.848	28.432	1.00 20.02	
	MOTA	1890	CB	ALA	A	309	28.056	23.856	27.106	1.00 18.80	
50	MOTA	1891	С	ÀLA	A	309	29.481	25.191	28.662	1.00 21.43	
	MOTA	1892	0	ALA	A	309	30.680	25.335		1.00 21.3	
	MOTA	1893	N	ARG	Α	310	28.717	26.179		1.00 21.3	
	MOTA	1894	CA	ARG	Α	310	29.290			1.00 22.03	
	MOTA	1895	CB			310	28.213			1.00 22.3	
55	MOTA	1896	CG	ARG	Α	310	28.806			1.00 25.3	
	MOTA	1897	CD	ARG	A	310	27.780			1.00 28.3	
	MOTA	1898	NE			310	28.420			1.00 30.1	
	MOTA	1899	cz			310	27.901			1.00 32.0	
	MOTA	1900	NH1	ARG	A	310	26.719	33.477	30.634	1.00 31.1	9 A

	ATOM	1901	NH2	ARG A	310	28.567	34.277	31.742	1.00 30.49	A
	MOTA	1902	С	ARG A	310	30.376	27.388	30.458	1.00 21.65	A
	MOTA	1903	0	ARG A	310	31.464	27.949	30.311	1.00 20.36	A
	ATOM	1904	N	ASP A	311	30.074	26.677	31.541	1.00 19.57	Α
5	ATOM	1905	CA	ASP A	311	31.043	26.512	32.615	1.00 20.18	A
	ATOM	1906	CB	ASP A	311	30.460	25.649	33.739	1.00 -20.39	A.
	MOTA	1907	CG	ASP A	311	31.439	25.446	34.881	1.00 23.35	A
	ATOM	1908	OD1	ASP A	311	32.158	24.428	34.885	1.00 24.91	A
	ATOM	1909	OD2	ASP A	311	31.500	26.312	35.776	1.00 26.96	A
10	MOTA	1910	C	ASP A	311	32.322	25.877	32.073	1.00 19.73	A
	MOTA	1911.	0	ASP A	311	33.422	26.289	32.439	1.00 19.30	Α
	ATOM	1912	N	LEU A	312	32.179	24.891	31.188	1.00 16.32	A
	MOTA	1913	CA	LEU A	312	33.349	24.226	30.611	1.00 16.66	A
	MOTA	1914	CB	LEU A		32.927	23.035	29.744	1.00 16.12	A
15	ATOM	1915	CG	LEU A	312	34.050	22.320	28.974	1.00 14.73	A
	ATOM	1916	CD1	LEU A	312	35.192	21.935	29.912	1.00 14.56	A
	MOTA	1917	CD2	LEU A	312	33.477	21.084	28.289	1.00 14.22	A
	MOTA	1918	C	LEU A	312	34.181	25.189	29.774	1.00 16.61	A
	MOTA	1919	0	LEU A	312	35.402	25.241	29.910	1.00 16.20	A
20	ATOM	1920	N	VAL A	313	33.515	25.949	28.908	1.00 16.20	A
	MOTA	1921	CA	VAL A	313	34.207	26.907	28.058	1.00 15.37	A
	ATOM	1922	CB	VAL A	313	33.216	27.648	27.130	1.00 16.42	A
	ATOM	1923	CG1	VAL A	313	33.915	28.796	26.426	1.00 16.93	A
	ATOM	1924	CG2	VAL A	313	32.644	26.672	26.103	1.00 17.88	A
25	MOTA	1925	С	VAL A	313	34.960	27.923	28.911	1.00 17.39	Α
	ATOM	1926	0	VAL A	313	36.093	28.294	28.591	1.00 18.00	Α
	MOTA	1927	N	GLU A	314	34.342	28.364	30.004	1.00 17.61	A
	MOTA	1928	CA	GLU A	314	34.986	29.331	30.885	1.00 20.43	A
	MOTA	1929	CB	GLU A	314	34.009	29.816	31.959	1.00 22.14	A
30	ATOM	1930	CG	GLU A	314	32.800	30.550	31.396	1.00 26.52	Α
	MOTA	1931	CD	GLU A	314	31.852	31.025	32.478	1.00 31.26	A
	MOTA	1932	OE1	GLU A	314	31.580	30.246	33.417	1.00 33.48	A
	MOTA	1933	OE2	GLU A	314	31.370	32.173	32.387	1.00 34.81	A
	MOTA	1934	С	GLU A	314	36.217	28.721	31.539	1.00 19.15	Α
35	MOTA	1935	0	GLU A	314	37.134	29.433	31.934	1.00 21.47	A
	MOTA	1936	N	LYS A	315	36.245	27.400	31.651	1.00 19.51	Α
	MOTA	1937	CA	LYS A	315	37.394	26.749	32.258	1.00 19.17	A
	MOTA	1938	CB	LYS A	315	36.946	25.514	33.043	1.00 18.84	A
	MOTA	1939	CG	LYS A	315	36.280	25.885	34.368	1.00 19.62	A
40	MOTA	1940	$^{\rm CD}$	LYS A	315 ·	35.653	24.696	35.073	1.00 19.22	A
	MOTA	1941	CE	LYS	315	35.070	25.095	36.427	0.50 21.00	AC1
	MOTA	1942	NZ	LYS	315	36.119	25.552	37.381	0.50 19.53	ACl
	MOTA	1943	C	LYS A	315	38.452	26.393	31.218	1.00 18.96	A
	MOTA	1944	0	LYS A	315	39.511	25.873	31.561	1.00 19.85	A
45	MOTA	1945	N	LEU A	316	38.164	26.691	29.950	1.00 17.08	A
	MOTA	1946	CA	LEU A	316	39.102	26.429	28.854	1.00 16.41	A
	ATOM	1947	CB	LEU A	316	38.414	25.636	27.738	1.00 13.81	Α
	ATOM	1948	CG	LEU A	316	38.028	24.201	28.115	1.00 14.39	A
	MOTA	1949	CD1	LEU A	316	37.139	23.597	27.031	1.00 12.38	Α
50	ATOM	1950	CD2	LEU A	316	39.302	23.373	28.309	1.00 12.77	A
	ATOM	1951	C	LEU A	316	39.652	27.743	28.290	1.00 17.12	Α
	ATOM	1952	0	LEU A	316	40.851	27.860	28.023	1.00 16.53	A
	ATOM	1953	N	LEU A	317	38.780	28.729	28.105	1.00 16.27	A
	ATOM	1954	CA	LEU A	317	39.228	30.022	27.596	1.00 17.52	A
55	MOTA	1955	CB	LEU A	317	38.083	30.752	26.887	1.00 16.37	A
	ATOM	1956	CG	LEU A	. 317	37.448	29.973	25.727	1.00 18.81	A
	MOTA	1957	CD1	LEU A	317	36.415	30.851	25.018	1.00 16.47	A
	ATOM	1958		LEU A		38.528	29.526	24.741	1.00 17.87	A
	MOTA	1959	C	LEU A	317	39.745	30.841	28.774	1.00 18.27	A

	ATOM	1960	0	LEU	Α	317	39	.078	31.753	2	9.273	1.00	18.58	A
	ATOM	1961	N	VAL	A	318	40	.937	30.475	2	9.229	1.00	18.02	A
	MOTA	1962	CA	VAL	Α	318	41	.593	31.141	. 3	0.342	1.00	18.85	A
	MOTA	1963	CB	VAL	Α	318	41	.846	30.153	3	1.500	1.00	19.91	A
5	MOTA	1964	CG1	VAL	Α	318	42	.590	30.848	3	2.634	1.00	20.01	A
	MOTA	1965	CG2	VAL	Α	318	40	.520	29.584	1 3	1.990		19.44	A
	ATOM	1966	C	VAL	A	318	42	.923	31.657	7 2	9.811		19.67	A
	MOTA	1967	0	VAL	Α	318	43	.690	30.902	2 2	9.208	1.00	18.26	A
	MOTA	1968	N	LEU	Α	319	43	.197	32.939		0.028		20.07	A
10	MOTA	1969	CA	LEU	Α	319	44	.436	33.533	3 2	9.538		20.98	A
	MOTA	1970	CB	LEU	Α	319	44	.521	35.002	2 2	9.968		21.64	A
	MOTA	1971	CG	LEU	A	319	43	.418	35.908		9.408		24.38	A
	ATOM	1972	CD1	LEU	Α	319	43	.606	37.332		9.935		23.28	Α.
	ATOM	1973	CD2	LEU	Α	319		.453	35.887		7.875		24.33	A
15	ATOM	1974	C	LEU	A	319	45	.680	32.774		9.994		20.38	A
	ATOM	1975	0	LEU	A	319		.568	32.496		9.192		21.34	A
	MOTA	1976	N	ASP	A	320		.742	32.440		1.280		20.22	A
	MOTA	1977	CA	ASP				.879	31.707		1.833		20.90	A
	MOTA	1978	CB	ASP				.842	31.760		3.365		20.76	A
20	MOTA	1979	CG	ASP				.049	31.102		4.004		21.51	A
	ATOM	1980		ASP				.669	30.226		33.367		23.46	A
	MOTA	1981		ASP				.371	31.450		5.159		23.89	A
	MOTA	1982	С	ASP				.814	30.247		1.367		20.06	A
	MOTA	1983	0	ASP				.988	29.476		11.840		20.54	A
25	MOTA	1984	N	ALA				.700	29.876		30.451		20.68	A
	MOTA	1985	CA	ALA				.733	28.522		9.903		22.04	A A
	MOTA	1986	CB	ALA				.860	28.411		28.881		20.75	A
	ATOM	1987	C	ALA				.858	27.400		30.940		21.02	A
	ATOM	1988	0	ALA				.482	26.259		30.665		20.89	A
30	ATOM	1989	N			322		3.372	27.715		32.127 33.167		20.83	A
	ATOM	1990	CA			322		.531	26.698		34.146		19.47	A
	ATOM	1991	CB			322).670).341	27.051 28.253		34.848		20.19	A
	ATOM	1992		THR THR				.981	27.249		33.394		21.59	A
25	MOTA	1993	CGZ			322		.264	26.498		33.983		19.55	A
35	MOTA	1994 1995	0	•		322		.235	25.673		34.894		21.13	A
	ATOM	1996	N			323		.216	27.248		33.661		19.33	A
	ATOM ATOM	1997	CA			323		.962	27.122		34.392		21.20	Ά
	ATOM	1998	CB			323		.580	28.460		35.030		23.75	A
40	ATOM	1999	CG			323		.562	28.933		36.084		28.45	A
70	ATOM	2000	CD			323		.055	30.17		36.799	1.00	33.76	A
	ATOM	2001	CE			323		.087	30.67		37.802	1.00	36.15	A
	ATOM.	2002	NZ			323		5.532	29.569		38.693	1.00	37.34	A
	ATOM	2003	C			323		.806	26.614		33.539	1.00	20.68	A
45	ATOM	2004	Ö			323	42	.649	26.75	7 :	33.915	1.00	20.42	A
	ATOM	2005	N			324		.114	26.01		32.392	1.00	19.97	A
	ATOM	2006	CA			324		.060	25.49	4 :	31.531	1.00	17.98	A
	ATOM	2007	CB			324		3.461	25.60	9 :	30.061	1.00	15.95	A
	ATOM	2008	CG	ARG	Α	324	43	3.534	27.05	0 :	29.603	1.00	17.34	A
50	MOTA	2009	CD	ARG	Α	324	43	.996	27.19	4	28.172		19.80	Α
	MOTA	2010	NE	ARG	Α	324	4.4	.438	28.56	5	27.944		16.93	A
	MOTA	2011	cz	ARG	A	324	45	5.410	28.90	8	27.108		19.88	Α
	MOTA	2012	NHl	ARG	A	324	46	5.045	27.97		26.398		14.58	A
	MOTA	2013	NH2	ARG	Α	324		5.774	30.18		27.015		16.51	A
55	MOTA	2014	C,	ARG	Α	324		2.762	24.04		31.883		18.32	A
	MOTA	2015	0	ARG	A	324	43	3.673	23.22		32.006		18.20	A
	MOTA	2016	N			325		L.479	23.74		32.055		18.32	A
	MOTA	2017	CA			325		L.050	22.40		32.395		17.79	
	MOTA	2018	CB	TEU	A	325	3 9	9.523	22.33	5	32.425	1.00	17.03	A

	MOTA	2019	CG	LEU	A	325	38.896	21.125	33.116	1.00 1	5.91	A
	ATOM	2020	CD1	LEU	Α	325	39.392	21.048	34.557	1.00 1	5.93	A
	ATOM	2021	CD2	LEU	Α	325	37.375	21.255	33.084	1.00 1	5.56	Α
	ATOM	2022	C	LEU	Α	325	41.599	21.433	31.356	1.00 1	3.68	A
5	MOTA	2023	0	LEU	Α	325	41.347	21.586	30.157	1.00 1		A
	MOTA	2024	N	GLY	Α	326	42.354	20.439	31.821	1.00 1	3.18	A
	ATOM	2025	CA			326	42.931	19.462	30.915	1.00 1		Α
	ATOM	2026	С	GLY	Α	326	44.443	19.558	30.807	1.00 1		A
	ATOM	2027	0			326	45.093	18.592	30.404	1.00 1		A
10	ATOM	2028	N			327	45.016	20.708	31.161	1.00 1		Α
	ATOM	2029	CA			327	46.463	20.867	31.075	1.00 1		Α
	ATOM	2030	CB			327	46.856	22.350	31.058	1.00 2		A
	ATOM	2031	SG			327	46.782	23.200	32.649	1.00 2		A
	ATOM	2032	С			327	47.169	20.157	32.228	1.00 2		A
15	ATOM	2033	0			327	46.561	19.828	33.246	1.00 1		A
	ATOM	2034	N		•	328	48.463	19.933	32.053	1.00 2		A
	ATOM	2035	CA			328	49.274	19.244	33.042	1.00 2		A
	ATOM	2036	CB			328	50.710	19.139	32.507	1.00 2		A
	ATOM	2037	CG			328	50.754	18.367	31.175	1.00 3		. A
20	ATOM	2038	CD			328	52.067	18.500	30.414	1.00 4		A
	MOTA	2039		GLU			52.535	19.643	30.218	1.00 4		A
•	ATOM	2040		GLU			52.618	17.459	29.991	1.00 4		A
	MOTA	2041	C			328	49.234	19.876	34.435	1.00 2		A
	ATOM	2042	0			328	49.147	19.161	35.437	1.00 2		A
25	ATOM	2043	И			329	49.276	21.204	34.506	1.00 1		A
	ATOM	2044	CA			329	49.248	21.875	35.801	1.00 2		A
	MOTA	2045	CB			329	49.587	23.363	35.657	1.00 2		A
	ATOM	2046	CG			329	51.014	23.651	35.190	1.00 2		A
20	ATOM	. 2047	CD			329	51.191	23.518	33.688	1.00 2		. A
30	MOTA	2048		GLU			50.213	23.154	32.995	1.00 2		A A
	MOTA	2049	-	GLU			52.311	23.781	33.198	1.00 2		A
	MOTA	2050	C			329	47.890 47.775	21.718	36.480	1.00 1		A
	MOTA	2051	N O			329 330		21.879	37.694	1.00 1		A
35	ATOM ATOM	2052 2053	CA			330	46.863 45.520	21.415 21.220	35.691 36.229	1.00 1		A
33	ATOM	2053	CB			330	44.474	21.220	35.294	1.00 1		A
	ATOM	2054	CG			330	44.460	23.365	35.311	1.00 1	1	A
	ATOM	2056	SD			330	44.186	24.026	36.979	1.00 2		A
	ATOM	2057	CE			330	42.435	23.712	37.186	1.00 2		A
40	ATOM	2058	C			330	45.257	19.730	36.422	1.00 1		A
••	ATOM	2059	o	MET			44.127	19.304	36.629	1.00 1		A
	ATOM	2060	N			331	46.327	18.949	36.346	1.00 1		A
	ATOM	2061	CA.			331	46.289	17.501	36.531	1.00 1		A
	ATOM	2062	СВ			331	45.607	17.155	37.862	1.00 1		A
45	MOTA	2063	CG			331	46.070	18.027	39.038	1.00 1	7.46	A
_	ATOM	2064	CD			331	47.591	18.179	39.145	1.00 2		A
	ATOM	2065		GLU	Α	331	48.034	19.073	39.896	1.00 2		A
	ATOM	2066		GLU			48.345	17.420	38.500	1.00 1		A
	ATOM	2067	C			331	45.697	16.658	35.398	1.00 1		A
50	ATOM	2068	0	GLU	Α	331	45.107	15.602	35.636	1.00 2	0.40	A
	ATOM	2069	N	GLY	Α	332	45.844	17.133	34.167	1.00 1	6.23	A
	ATOM	2070	CA			332	45.420	16.353	33.015	1.00 1	4.10	A
	MOTA	2071	C	GLY	A	332	43.982	16.154	32.596	1.00 1	3.54	A
	MOTA	2072	0	GLY	A	332	43.063	16.864	33.017	1.00 1		A
55	MOTA	2073	N	TYR	A	333	43.804	15.141	31.750	1.00 1		A
	MOTA	2074	CA	TYR	A	333	42.510	14.806	31.182	1.00 1		A
	MOTA	2075	CB	TYR	A	333	42.722	13.892	29.968	1.00 1		A
	MOTA	2076	CG			333	43.153	14.683	28.752	1.00 1	6.46	A
	ATOM	2077	CD1	TYR	Α	333	42.206	15.172	27.849	1.00 1	5.29	A

•	ATOM	2078	CE1	TYR	Α	333		42.	. 573	16.	002	26.7	94		13.42	
	ATOM	2079	CD2	TYR	Α	333		44.	.490	15.	039	28.5	51		14.91	
	MOTA	2080	CE2	TYR	Α	333		44	.872	15.	877	27.4	99		14.87	
	MOTA	2081	CZ	TYR	Α	333		43	. 902	16.		26.6			15.61	
5	MOTA	2082	OH	TYR	A	333		44	.244	17.	197	25.5			17.29	
	MOTA	2083	C	TYR	Α	333		41	.470	14.		32.1			15.23	
	MOTA	2084	0	TYR	Α	333		40	.278	14.	323	31.8			16.63	
	MOTA	2085	N	GLY	Α	334		41	.907	13.	650	33.2	44		15.50	
	MOTA	2086	CA	GLY	Α	334		40	. 957	13.	100	34.2			15.07	
10	MOTA	2087	C	GLY	Α	334		39	. 925	14.	146	34.6			16.40	
	MOTA	2088	0	GLY	Α	334		38	.724	13.	946	34.4			15.05	
	MOTA	2089	N	PRO	Α	335		40	.366	15.	278	35.1			14.96	
	MOTA	2090	CD	PRO	Α	335		41	.727	15.	531	35.6	89		15.88	
	MOTA	2091	CA	PRO	Α	335		39	.444	16.	339	35.6	06		15.29	
15	MOTA	2092	CB	PRO	Α	335		40	.383	17.	397	36.1	78		13.19	
	MOTA	2093	CG	PRO	Α	335		41	.485	16.	569	36.7	58		13.81	
•	MOTA	2094	С	PRO	A	335		38	.594	16.	877	34.4	48		15.84	
	ATOM	2095	0	PRO	Α	335		37	.423	17.	204	34.6	31		14.84	
	ATOM	2096	N	LEU	A	336		39	.184	16.	971	33.2	57		16.12	
20	MOTA	2097	CA	LEU	Α	336		38	.450	17.	465	32.0	94		15.52	
	MOTA	2098	CB	LEU	Α	336		39	.396	17.	653	30.8	98		14.39	
	MOTA	2099	CG	LEU	Α	336	•	38	.770	17.	991	29.5	38		15.46	
	MOTA	2100	CD1	LEU	A	336		37	.836	19.	182	29.6	62		11.25	
	MOTA	2101	CD2	LEU	A	336		39	.884	18.	285	28.5	28		14.11	
25	MOTA	2102	C	LEU	А	336		37	.321	16.	508	31.7	14		16.28	
	MOTA	2103	0	LEU	А	336		36	.176	16.	921	31.5	40		15.51	
	ATOM	2104	N	LYS	Α	337		37	.640	15.	225	31.5	92	1.00	17.22	
	MOTA	2105	CA	LYS	Α	337		36	.624	14.	243	31.2	35		17.39	
	MOTA	2106	CB	LYS	A	337		37	.293	12.	900	30.9	21		17.68	
30	MOTA	2107	CG	LYS	А	337		38	.170	12.	994	29.6			22.31	
	ATOM	2108	CD	LYS	Α	337		39	.213	11.	892	29.5	92		24.60	
	ATOM	2109	CE	LYS	A	337		38	.620	10.	560	29.1			24.76	
	MOTA	2110	NZ	LYS	A	337		39	.710	9.	560	28.9			25.05	
	MOTA	2111	C	LYS	A	337		35	.577	14.	096	32.3			17.33	
35	MOTA	2112	0	LYS	Α	337		34	.456	13.	652	32.0			14.42	
	ATOM	2113	N	ALA	A	338		35	.928	14.	500	33.5			15.83	
	MOTA	2114,	CA	ALA	А	338		34	.989	14.	395	34.6			17.52	
	MOTA	2115	CB	ALA	A	338		35	.749	14.	167	35.9	80		19.68	
	MOTA	2116	C	ALA	A	338		34	.095	15.	621	34.8			18.83	
40	MOTA	2117	0	ALA	A	338		33	. 252		687	35.6			18.94	
	MOTA	2118	N	HIS	A	339		34	.262		596	33.9			19.42	
	ATOM	2119	CA	HIS	A	339		33	.438		796	34.0			19.28	
	MOTA	2120	CB	HIS	A	339			.865		819	32.9			19.20	
	ATOM	2121	CG			339			.163		134	33.0			20.26	_
45	ATOM	2122		HIS					.549		299	33.6			0 18.9	
	MOTA	2123		HIS					.880		340	32.6	•		0 19.10	
	MOTA	2124	CE1	HIS	A	339			.506		576	32.8			0 22.19	
	MOTA	2125	NE2	HIS					.500		179	33.5			0 21.9	
	MOTA	2126	C			339			.957		448	33.8			0 19.13	
50	MOTA	2127	0			339			.597		576	33.0			0 19.5	
	MOTA	2128	N			340			.079		125	34.6			0 19.8	
	MOTA	2129	CD			340			.424		119	35.6			0 19.0	
	MOTA	2130	CA			340			.630		900	34.5			0 20.5	
	MOTA	2131	CB			340			.091		.058	35.3			0 20.7	
55	ATOM	2132	CG			340			.146		.207	36.4			0 19.2	
	MOTA	2133	C			340			.000		. 834	33.1			0 21.4	
	MOTA	2134	0			340			.049		. 088	32.9			0 22.4	
	MOTA	2135	N			341			.528		.606	32.2			0 21.3	
	MOTA	2136	CA	PHE	A	341		28	.985	18	.610	30.8	386	1.0	0 21.5	7 A

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	ATOM	2137	СВ	PHE A	341	29.739	19.624	30.017	1.00 21.64	A
	MOTA	2138	CG	PHE A	341	29.207	19.740	28.613	1.00 23.18	A
	ATOM	2139	CD1	PHE 2	341	27.903	20.171	28.382	1.00 22.58	A
	ATOM	2140	CD2	PHE A	341	30.013	19.431	27.522	1.00 21.95	A
5	ATOM	2141	CE1	PHE A	A 341	27.410	20.292	27.082	1.00 23.54	A
	ATOM	2142	CE2	PHE A	4 341	29.533	19.548	26.220	1.00 21.83	A
	ATOM	2143	CZ		341	28.228	19.980	25.998	1.00 23.23	A
	ATOM	2144	C		A 341		17.226	30.237	1.00 21.84	Α
	ATOM	2145	ō		341		16.896	29.389	1.00 20.37	A
10	ATOM	2146	N		A 342		16.422	30.640	1.00 20.51	A
•	ATOM	2147	CA		A 342		15.085	30.077	1.00 23.01	Α
	ATOM	2148	CB		A 342		14.809	29.850	1.00 18.00	A
	ATOM	2149	CG		A 342		15.812	28.971	1.00 17.05	A
	ATOM	2150		PHE A			15.987	27.652	1.00 17.78	A
15				PHE			16.534	29.450	1.00 17.70	A
15	ATOM	2151					16.867	26.811	1.00 18.08	A
	ATOM	2152		PHE		•	17.414	28.617	1.00 10.00	A
	ATOM	2153		PHE A			17.578	27.298	1.00 17.45	A
	ATOM	2154	CZ		A 342				1.00 10.30	A
20	ATOM	2155	C		A 342		13.972	30.976	1.00 24.95	A
20	ATOM	2156	0		A 342		12.798	30.777		
	MOTA	2157	N		A 343		14.333	31.958	1.00 27.35	A
	MOTA	2158	CA		A 343		13.349	32.897	1.00 30.28	A
	MOTA	2159	CB		A 343		13.964	33.716	1.00 32.20	A
	MOTA	2160	CG		A 343		12.991	34.714	1.00 39.71	A
25	ATOM	2161	CD		A 343	-	13.661	35 688	1.00 44.72	A
	ATOM	2162		GLU .			14.314	35.234	1.00 47.55	A
	ATOM	2163		GLU .			13.526	36.911	1.00 46.89	A
	ATOM	2164	С		A 343		12.017	32.305	1.00 28.98	A
	MOTA	2165	0		A 343		10.952	32.800	1.00 31.73	A
30	ATOM	2166	И		A 344		12.067	31.258	1.00 26.09	A
	ATOM	2167	CA	SER .	A 344	26.520	10.838	30.656	1.00 28.36	A
	ATOM	2168	CB	SER .	A 344		11.089	30.067	1.00 28.73	Α
	ATOM	2169	OG	SER .	A 344	25.203	11.942	28.940	1.00 30.91	A
	MOTA	2170	C	SER .	A 344	27.407	10.214	29.577	1.00 27.66	Α
35	ATOM	2171	Ο.	SER .	A 344	26.987	9.281	28.900	1.00 28.66	A
	ATOM	2172	N	VAL .	A 345	28.627	10.715	29.419	1.00 26.75	A
	ATOM	2173	CA	VAL .	A 345	29.534	10.183	28.402	1.00 23.44	A
	MOTA	2174	CB	VAL .	A 345	30.565	11.256	27.950	1.00 23.10	Α
	ATOM	2175	CG1	VAL .	A 345	. 31.589	10.631	26.995	1.00 22.24	A
40	ATOM	2176	CG2	VAL .	A 345	29.854	12.418	27.275	1.00 20.05	Ą
	MOTA	2177	С	VAL .	A 345	30.326	8.957	28.855	1.00 24.26	A
	ATOM	2178	0	VAL .	A 345	30.876	8.930	29.960	1.00 22.83	A
	ATOM	2179	N	THR .	A 346	30.374	7.942	27.997	1.00 21.77	A
	ATOM	2180	CA	THR	A 346	31.153	6.740	28.272	1.00 23.70	A
45	MOTA	2181	CB	THR	A 346	30.391	5.455	27.857	1.00 26.53	Α
	ATOM	2182	OG1	THR	A 346	29.248	5.284	28.706	1.00 29.98	A
	ATOM	2183	CG2	THR	A 346	31.289	4.231	27.990	1.00 24.28	Α.
	ATOM	2184	C	THR	A 346	32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	0	THR	A 346	32.306	6.827	26.160	1.00 24.50	Α
50	ATOM	2186	N	TRP	A 347		7.270	28.013	1.00 22.98	A
	ATOM	2187	CA	TRP	A 347	34.744	7.569	27.300	1.00 23.81	A
	ATOM	2188	СВ		A 347		8.352	28.219	1.00 22.54	A
	ATOM	2189	CG		A 347		9.658	28.693	1.00 20.61	A
	ATOM	2190		TRP			10.927	28.040	1.00 19.11	A
55	ATOM	2191	CE2		A 347		11.881	28.838	1.00 18.39	A
	ATOM	2192		TRP			11.351	26.858	1.00 18.16	A
	ATOM	2193		TRP			9.883	29.828	1.00 18.35	A
	ATOM	2194		TRP			11.218	29.923	1.00 19.51	A
	ATOM	2195		TRP			13.234	28.491	1.00 16.88	A

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	ATOM .	2196	CZ3	TRP	A:	347	35.808	12.701	26.511	1.00 17.23	A
	MOTA	2197	CH2	TRP	Α	347	35.127	13.624	27.327	1.00 18.16	A
	ATOM	2198	C	TRP	Α	347	35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	0	TRP	Α	347	36.304	6.654	25.742	1.00 24.67	A
5	MOTA	2200	N	ALA	Α	348	35.360	5.215	27.183	1.00 27.10	A
_	ATOM	2201	CA	ALA	A	348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	СВ	ALA	Α	348	35.899	2.869	27.636	1.00 27.09	A
	ATOM	2203	C	ALA	А	348	35.895	3.620	25.256	1.00 27.18	A
	ATOM	2204	ō	ALA			36.830	3.148	24.613	1.00 29.41	A
10	ATOM	2205	N	ASN			34.682	3.769	24.735	1.00 26.55	Α
	ATOM	2206	CA	ASN			34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	CB	ASN			33.700	1.962	23.444	1.00 29.37	A
	ATOM	2207	CG	ASN			32.299	2.088	24.013	1.00 30.92	A
				ASN			32.045	2.942	24.859	1.00 30.17	A
1.5	ATOM	2209		ASN			31.386	1.237	23.553	1.00 33.52	A
15	MOTA	2210		ASN			33.599	4.265	22.509	1.00 26.47	A
	ATOM	2211	C	ASN			32.669	3.843	21.819	1.00 25.87	A
	MOTA	2212	0				33.947	5.543	22.518	1.00 24.45	A
	MOTA	2213	N	LEU				6.510	21.721	1.00 23.14	A
	MOTA	2214	CA	LEU			33.203		21.721	1.00 23.22	A
20	MOTA	2215	CB	LEU			33.837	7.898	23.191	1.00 23.22	. A
	MOTA	2216	CG	LEU			33.659	8.605		1.00 21.05	A
,	ATOM	2217		LEU			34.646	9.756	23.293	1.00 19.30	A
	MOTA	2218		LEU			32.220	9.094	23.319	1.00 18.78	A
	MOTA	2219	С	LEU			33.082	6.152	20.240		A
25	ATOM	2220	0	LEU			32.011	6.296	19.650	1.00 21.15	A
	MOTA	2221	N	HIS			34.165	5.689	19.627	1.00 23.13	A
	MOTA	2222	CA	HIS			34.089	5.387	18.204	1.00 27.83	
	MOTA	2223	CB	HIS			35.506	5.325	17.596	1.00 29.36	A
•	MOTA	2224	CG	HIS			36.082	3.950	17.493	1.00 32.07	A
30	MOTA	2225		HIS			36.611	3.128	18.431	1.00 32.39	A
	MOTA	2226	NDl	HIS	Α	351	36.197	3.285	16.291	1.00 33.02	· A
	MOTA	2227		HIS			36.775	2.113	16.493	1.00 33.58	A
	MOTA	2228	NE2	HIS	A	351	37.036	1.992	17.782	1.00 31.76	A
	MOTA	2229	C	HIS	Α	351	33.258	4.144	17.874	1.00 28.12	A
35	MOTA	2230	0	HIS	Α	351	33.015	3.847	16.707	1.00 29.49	A
	MOTA	2231	N	GLN	A	352	32.800	3.442	18.908	1.00 29.28	A
	MOTA	2232	CA	GLN	Α	352	31.963	2.255	18.726	1.00 29.67	Α
	MOTA	2233	CB	GLN		352	32.366	1.145	19.694	0.50 30.56	AC1
	MOTA	2234	CG	GLN		352	33.169	0.041	19.041	0.50 30.88	AC1
40	ATOM	2235	CD	GLN		352	34.493	-0.186	19.729	0.50 31.21	AC1
	ATOM	2236	OE1	GLN		352	34.541	-0.450	20.928	0.50 30.76	AC1
	ATOM	2237	NE2	GFM		352	35.578	-0.084	18.971	0.50 32.30	AC1
	ATOM	2238	С	GLN	Α	352	30.504	2.638	18.963	1.00 30.42	A
	ATOM	2239	0	GLN	Α	352	29.595	1.831	18.770	1.00 29.01	A
45	ATOM	2240	N	GLN	Α	353	30.290	3.875	19.397	1.00 27.64	A
	ATOM	2241	CA			353	28.948	4.365	19.652	1.00 27.42	A
	ATOM	2242	CB			353	28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG			353	29.408	4.837	22.115	1.00 27.34	A
	ATOM	2244	CD			353	29.638	5.914	23.156	1.00 27.19	A
50	ATOM	2245		GLN			28.875	6.872	23.252	1.00 28.29	A
50	ATOM	2246		GLN			30.687	5.753	23.951	1.00 28.79	A
	ATOM	2247	C			353	28.375	4.989	18.385	1.00 29.00	A
	ATOM	2248	ō			353	29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N			354	27.053	4.984	18.276	1.00 27.31	A
55	ATOM	2250	CA			354	26.390		17.119	1.00 27.85	A
"	MOTA	2251	CB			354	24.991	4.941	16.904	1.00 30.69	A
		2252		THR			25.132	3.532	16.665	1.00 30.07	A
	MOTA	2252		THR			24.289		15.709	1.00 29.58	A
	ATOM		C			354	26.244	7.062	17.376	1.00 26.85	A
	MOTA	2254	_	TUK	· A	コンエ	20.633		_,,,,,,		

	ATOM	2255	0	THR	A	354	25.592	7.475	18.329	1.00 25.77	A
	ATOM	2256	N	PRO	Α	355	26.867	7.898	16.533	1.00 27.22	A
	ATOM	2257	CD	PRO	Α	355	27.792	7.588	15.431	1.00 25.89	A
	ATOM	2258	CA	PRO	A	355	26.763	9.346	16.734	1.00 27.23	A
5	ATOM	2259	CB	PRO	A	355	27.625	9.915	15.609	1.00 24.91	A
	ATOM	2260	CG	PRO	A	355	28.643	8.838	15.385	1.00 25.54	A
	ATOM	2261	С	PRO	A	355	25.322	9.837	16.641	1.00 28.07	A
	ATOM	2262	0	PRO	Α	355	24.548	9.364	15.810	1.00 27.24	A
	ATOM	2263	N	PRO	Α	356	24.941	10.792	17.500	1.00 28.28	A
10	ATOM	2264	CD	PRO	A	356	25.752	11.560	18.462	1.00 28.31	A
	ATOM	2265	CA	PRO	A	356	23.572	11.306	17.448	1.00 28.44	A
	ATOM	2266	CB	PRO	A	356	23.539	12.301	18.604	1.00 28.11	A
	ATOM	2267	CG	PRO	Α	356	24.946	12.832	18.612	1.00 26.86	A
	ATOM	2268	C	PRO	Α	356	23.363	11.978	16.097	1.00 29.25	A
15	MOTA	2269	0	PRO	A	356	24.304	12.537	15.529	1.00 27.27	A
	ATOM	2270	N	ALA	Α	357	22.143	11.910	15.575	1.00 30.45	A
	MOTA	2271	CA	ALA	A	357	21.848	12.521	14.287	1.00 32.81	· A
	ATOM	2272	CB	ALA	А	357	20.507	12.019	13.757	1.00 31.99	A
	MOTA	2273	C	ALA	A	357	21.824	14.035	14.448	1.00 35.05	A
20	MOTA	2274	0	ALA	A	357	21.194	14.561	15.369	1.00 35.04	A
	ATOM	2275	И	LEU	Α	358	22.516	14.730	13.552	1.00 37.81	A
	MOTA	2276	CA			358	22.578	16.185	13.597	1.00 42.15	A
	MOTA	2277	CB			358	23.679	16.681	12.658	1.00 39.54	A
	MOTA	2278	CG			358	25.086	16.285	13.109	1.00 39.51	A
25	MOTA	2279		LEU			26.102	16.686	12.062	1.00 39.29	A
	MOTA	2280		LEU			25.395	16.953	14.445	1.00 40.01	A
	MOTA	2281	С		-	358	21.241	16.837	13.242	1.00 45.91	A
	MOTA	2282	0			358	20.874	16.927	12.069	1.00 45.71	A
	ATOM	2283	N			359	20.530	17.290	14.275	1.00 50.06	A
30	MOTA	2284	CA			359	19.223	17.939	14.140	1.00 53.73	A
	ATOM	2285	CB			359	19.353	19.428	13.726	1.00 54.04	A
	ATOM	2286		THR			19.995	19.521	12.448	1.00 56.35	A
	ATOM	2287		THR			20.158	20.204	14.763	1.00 54.32	A
25	ATOM	2288	C			359	18.309	17.236	13.139	1.00 54.47	A
35	ATOM	2289	0 ,	THR			18.483	16.016	12.930	1.00 55.90	A
	ATOM	2290		THR			17.407	17.908	12.595	1.00 56.97	A S
	MOTA	2291		TIP		1	42.566	19.118	34.302	1.00 15.09	S
	MOTA	2292		TIP		2	41.052 37.014	32.378	19.857 17.747	1.00 15.82 1.00 16.95	S
40	ATOM	2293 2294	OH2	TIP TIP	S	3 5	45.353	33.030 24.370	18.152	1.00 16.95	S
40	ATOM ATOM	2295		TIP		6	31.896	13.930	33.235	1.00 10.03	S
	ATOM	2296	OH2			7	50.351	22.781	28.249	1.00 20.42	S
	ATOM	2297		TIP		8	45.246	-0.589	-0.734	1.00 21.14	S
	ATOM	2298	OH2	TIP		11	46.249	-0.348	-8.523	1.00 21.32	S
45	ATOM	2299		TIP		14	45.756	11.148	29.680	1.00 21.94	s
73	ATOM	2300		TIP		15	44.273	13.157	34.592	1.00 15.61	s
	ATOM	2301		TIP		17	53.598	3.722	-1.720	1.00 21.45	S
	ATOM	2302		TIP		18	46.049	13.087	31.565	1.00 20.35	S
	ATOM	2303		TIP		19	53.422	22.401	-3.280	1.00 23.26	s
50	ATOM	2304		TIP		20	34.587	7.922	5.383	1.00 22.58	S
50	ATOM	2305		TIP		21	45.053	27.379	19.376	1.00 29.60	S
	ATOM	2306		TIP		23	28.899	36.416	28.633	1.00 31.68	S
	ATOM	2307		TIP		24	35.531	11.645	-8.219	1.00 23.45	S
	ATOM	2308		TIP		25	47.364	28.787	19.612	1.00 23.03	s
55	ATOM	2309		TIP		27	48.859	21.588	12.634	1.00 23.76	S
	ATOM	2310		TIP		29	48.805	8.920	23.626	1.00 22.23	S
	ATOM	2311		TIP		31	48.619	7.247	10.112	1.00 21.32	S
	MOTA	2312		TIP		34	44.824	28.720	15.621	1.00 25.27	S
	MOTA	2313		TIP		35	26.030	12.634	13.407	1.00 21.61	S

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		•								
	MOTA	2314	OH2	TIP	S 36	50.462	19.810	40.066	1.00 25.45	S
	ATOM	2315	OH2	TIP	S 37	39.631	23.510	-0.239	1.00 30.88	S
	ATOM	2316	OH2	TIP	S 40	44.734	42.655	10.346	1.00 30.84	S
	ATOM	2317	OH2	TIP	S 41	54.653	3.902	1.503	1.00 27.14	S
5	MOTA	2318	OH2	TIP	S 45	45.693	21.923	39.754	1.00 28.30	S
	MOTA	2319	OH2	TIP	S 47	47.820	16.413	7.805	1.00 25.73	S
	MOTA	2320	OH2	TIP	S 48	50.292	31.412	29.642	1.00 32.79	S
	MOTA	2321	OH2	TIP	S 49	26.056	16.646	34.827	1.00 29.80	S
	MOTA	2322	OH2	TIP	S 52	31.714	10.996	31.855	1.00 29.15	S
10	MOTA	2323	OH2	TIP	S 53	46.108	23.843	-4.299	1.00 24.21	S
	MOTA	2324		TIP	5 54	37.645	11.206	34.448	1.00 28.56	S
	MOTA	2325			S 55		28.513	12.142	1.00 32.08	S
	MOTA	2326		TIP		•	19.700	3.483	1.00 28.28	S
	MOTA	2327		TIP			-0.632	14.280	1.00 32.13	S
15	MOTA	2328			S 65		26.036	34.324	1.00 24.17	S
	MOTA	2329		TIP			3.958	14.729	1.00 28.94	S
	MOTA	2330		TIP			11.604	6.814	1.00 38.35	S
	ATOM	2331		TIP			44.403	18.686	1.00 26.61	· S
20	MOTA	2332		TIP			12.366	27.366	1.00 28.51	S
20	MOTA	2333		TIP			33.771	33.329	1.00 28.82	S
	ATOM	2334			S 81		13.106	2.128	1.00 40.62	S
	ATOM	2335		TIP			34.381	32.043	1.00 19.35 1.00 21.14	s s
	MOTA MOTA	2336 2337			S 85 S 88		40.331	19.200 -6.556	1.00 21.14	S
25	ATOM	2338		TIP			-0.832 28.336	33.481	1.00 27.64	S
23	ATOM	2339		TIP			-7.101	-7.995	1.00 24.33	S
	ATOM	2340		TIP			4.387	19.370	1.00 24.33	S
	ATOM	2341		TIP			11.549	33.898	1.00 29.40	s
	ATOM	2342		TIP			24.831	1.168	1.00 26.53	s
30	MOTA	2343		TIP			4.952	-6.749	1.00 28.00	S
	ATOM	2344		TIP			27.986	11.558	1.00 29.24	S
	ATOM	2345		TIP			24.366	30.265	1.00 31.61	S
	MOTA	2346		TIP			7.113	-8.298	1.00 31.57	s
	MOTA	2347	OH2	TIP	S 102	58.318	19.957	-8.378	1.00 26.95	S
35 .	MOTA	2348	OH2	TIP	5 103	49.647	22.446	39.624	1.00 40.57	S
	MOTA	2349	OH2	TIP	S 104	45.359	7.052	13.052	1.00 26.27	S
	MOTA	2350	OH2		S 105		32.340	32.346	1.00 34.45	S
	MOTA	2351	OH2		S 107		40.457	8.240	1.00 40.48	S
	MOTA	2352	OH2			36.644	8.257	13.418	1.00 30.70	S
40	ATOM	2353		TIP		41.912	-8.974	-8.264	1.00 26.08	S
	ATOM	2354	OH2		S 124		15.800	-7.411	1.00 24.08	S
	ATOM	2355	OH2		S 126		18.656	-9.097	1.00 28.99	S
	MOTA	2356		TIP		43.129	26.845	14.606	1.00 25.19	S
46	MOTA	2357	OH2	TIP		36.339	32.639	29.802	1.00 29.25	- S
45	MOTA	2358		TIP			14.561	26.498	1.00 33.93	S
	ATOM	2359		TIP			-4.242	5.492	1.00 33.72	S
	ATOM	2360		TIP			25.163	36.697	1.00 30.69	S
	ATOM ATOM	2361 2362		TIP			8.553 10.546	25.307	1.00 31.43 1.00 33.45	s s
50	ATOM	2363		TIP TIP			15.434	11.467	1.00 33.45	S
50	ATOM ·			TIP		31.040	12.361	35.470	1.00 34.07	s
	ATOM	2365		TIP			14.292	-0.598	1.00 40.68	S
	ATOM	2366		TIP			8.748	11.662	1.00 29.23	s
	ATOM	2367		TIP		46.297	-7.287	-9.196	1.00 42.20	s
55	ATOM	2368		TIP		58.193	6.715	-4.685	1.00 35.48	s
	ATOM	2369		TIP			4.435	12.503	1.00 27.68	S
	MOTA	2370		TIP		27.003	5.999	12.450	1.00 36.30	s
	MOTA	2371	·OH2	TIP	S 145	43.676	32.852	35.735	1.00 35.70	s
	MOTA	2372		TIP			18.628	36.452	1.00 34.62	S

	ATOM	2373	OH2	TIP	s	147		25.402	4.058	20.638	1.00	45.03	S
	ATOM	2374	OH2					45.839	35.853	33.724		35.47	s
	ATOM	2375	OH2			149		22.176	18.976	16.752		31.87	· s
	ATOM	2376	OH2			150		43.986	33.179	10.162		37.70	s
5	ATOM	2377	OH2					50.653	20.347	42.428		35.80	s
,	ATOM	2378	OH2			152		47.843	24.314	9.506		31.05	s
		2379						44.693		-14.175		29.90	S
	ATOM		OH2	TIP		153							
	ATOM	2380	OH2	TIP				26.560	36.851	31.684		49.29	S
10	ATOM	2381	OH2					46.867		-12.951		29.21	s
10	ATOM	2382		TIP		157		30.432	28.741	12.438		37.76	S
•	ATOM	2383		TIP				41.004	20.553	6.423		39.53	S
	MOTA	2384		TIP				49.258	20.069	29.294		33.97	S
	ATOM	2385	OH2	TIP		160		48.082	28.459	,16.489		33.10	S
	MOTA	2386	OH2	TIP	S	161		47.448	18.625	27.683	1.00	34.87	S
15	ATOM	2387	OH2	TIP	S	162		19.687	20.632	23.411	1.00	35.01	S
	MOTA	2388	OH2	TIP	S	163		32.402	-1.266	22.443	1.00	37.26	s
	MOTA	2389	OH2	TIP	S	164		39.475	33.468	33.237	1.00	35.34	s
	ATOM	2390	OH2	TIP	S	165		44.277	18.950	5.162	1.00	45.14	S
	ATOM	2391	OH2	TIP	s	166		34.797	30.523	10.736	1.00	47.55	S
20	MOTA	2392	OH2	TIP	s	167		46.541	3.526	-14.949	1.00	26.54	s
	MOTA	2393	OH2	TIP		168		36.333	16.371	1.539	1.00	38.68	s
	MOTA	2394		TIP		169		46.761	38.936	27.403		34.66	s
	ATOM	2395	OH2	TIP		170		24.163	13.264	11.375		41.23	s
	ATOM	2396	OH2	TIP		171		48.459	15.018	31.951		38.11	S
25	ATOM	2397	OH2			172		34.261	23.193	40.004		48.96	S
23	ATOM	2398	OH2	TIP		173		45.924	-0.026	13.224		39.55	s
	MOTA	2399	OH2	TIP		175		41.384	37.389	32.543		40.74	S
	ATOM	2400		TIP		177		49.394	35.312	27.150		44.33	S
			OH2							34.359		41.46	S
20	ATOM	2401		TIP		178		29.066	29.942				S
30	ATOM	2402	OH2	TIP		180		49.354	19.467	7.273		34.56	
	ATOM	2403	OH2			181		25.298	17.029	31.863		47.74	S
	ATOM	2404	OH2	TIP		182		37.071	25.027	4.669		43.87	₂S
	ATOM	2405	OH2	TIP				22.581	7.487	18.691		41.75	S
	ATOM	2406		TIP		184		32.269	7.011	-1.891		48.84	S
35	ATOM	2407	OH2					48.234	0.494	6.833		48.16	
	ATOM	2408	OH2	TIP		187		20.008	14.658	19.211		45.27	S
	ATOM	2409	OH2	TIP		188		49.341	22.698	42.272		42.20	S
	MOTA	2410	OH2	TIP	S	190		61.292	18.260	-8.097		45.21	S
	ATOM	2411	OH2	TIP		191		28.152	10.606	2.819		40.38	s
40	MOTA	2412	OH2	TIP	S	192		25.626	12.619	23.191	1.00	34.27	s
	MOTA	2413	OH2	TIP	S	193		59.876	11.603	1.216	1.00	46.54	s
	MOTA	2414	OH2	TIP	S	194		57.592	21.183	-10.646	1.00	45.82	s
	ATOM	2415	OH2	TIP	S	195		31.509	36.649	21.499	1.00	38.73	·s
	ATOM	2416	OH2	TIP	S	197		50.270	-1.543	-6.136	1.00	42.66	S
45	ATOM	2417	OH2	TIP	s	198		24.467	8.729	13.088	1.00	42.78	S
	MOTA	2418	OH2	TIP	s	199		38.098	8:699	25.759	1.00	32.80	S
	ATOM	2419		TIP				57.831		-13.255	1.00	45.31	s
	ATOM	2420		TIP				23.888	22.328	30.524		37.12	S
	ATOM	2421		TIP				47.691	26.068	37.666		37.92	s
50	ATOM	2422		TIP			•	38.653	7.070	29.307		50.54	s
	ATOM	2423		TIP				44.424	27.583	2.092		53.50	s
	ATOM	2424		TIP				22.258	2.296	17.948		47.38	S
	ATOM	2425		TIP				19.843	17.943	23.303		30.36	s
	ATOM	2425		TIP				27.647	11.344	24.681		31.32	S
55	ATOM	2427		TIP			•	37.953	7.817	-9.284		45.97	s
23	ATOM	2427		TIP				37.953	34.040	12.124		38.11	S
													S
	ATOM	2429		TIP				58.484	15.269	13.717		38.26	S
	ATOM	2430		TIP				48.526	40.920	26.583		35.23	S
	ATOM	2431	OH2	TIP	S	222		52.094	21.184	38.122	T.00	29.86	3

		•						
	MOTA	2432	OH2 TIP S 22	36.889	5.881	3.281	1.00 37.63	S
	MOTA	2433	OH2 TIP S 22	24 . 47.642	-1.401	-10.684	1.00 34.89	S
	ATOM	2434	OH2 TIP S 22	26 47.284	2.916	19.133	1.00 34.10	S
	MOTA	2435	OH2 TIP S 22	42.468	4.463	-15.039	1.00 37.98	S
5	ATOM	2436	OH2 TIP S 22	19.169	22.832	21.831	1.00 41.57	S
	ATOM	2437	OH2 TIP S 23	57.592	12.689	14.880	1.00 50.22	S
	MOTA	2438	OH2 TIP S 23	32 27.102	9.176	5.655	1.00 40.57	S
	ATOM	2439	OH2 TIP S 23	33 58.618	9.072	-11.925	1.00 50.71	s
	MOTA	2440	OH2 TIP S 23	34 22.822	25.342	19.945	1.00 34.93	S
10	ATOM	2441	OH2 TIP S 2	36 24.831	32.218	28.901	1.00 37.69	S
	ATOM	2442	OH2 TIP S 23	37 20.045	10.774	16.992	1.00 39.57	S
	ATOM	2443	OH2 TIP S 2		19.850	15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP S 2	39 19.490	20.949	26.114	1.00 34.55	S
	ATOM	2445	OH2 TIP S 24	10 61.187	26.377	7.346	1.00 39.68	S
15	MOTA	2446	OH2 TIP S 2	11 33.680	38.342	19.389	1.00 48.93	S
	MOTA	2447	OH2 TIP S 2		31.612	10.881	1.00 55.65	S
	MOTA	2448	OH2 TIP S 2		14.431	30.404	1.00 46.69	S
	ATOM	2449	OH2 TIP S 2		5.849	9.544	1.00 43.81	S
	MOTA	2450	OH2 TIP S 2		-1.293	-9.655	1.00 42.96	. \$
20	MOTA	2451		58. 23.938	30.000	30.010	1.00 38.89	S
	MOTA	2452	OH2 TIP S 2			32.578	1.00 40.17	S
	ATOM	2453	OH2 TIP S 2		17.986	1.918	1.00 48.36	S
	ATOM	2454	OH2 TIP S 2		12.876	25.603	1.00 57.17	s s
	MOTA	2455	OH2 TIP S 2		36.767	12.550	1.00 30.70	
25	MOTA	2456	OH2 TIP S 2		25.529	30.131	1.00 44.85 1.00 37.15	S S
	ATOM	2457	OH2 TIP S 2			36.003	1.00 37.13	S
	ATOM	2458	OH2 TIP S 2			23.723 11.014	1.00 43.29	S
	MOTA	2459	OH2 TIP S 2			22.447	1.00 30.13	S
20	ATOM	2460	OH2 TIP S 2			10.235	1.00 37.91	S
30	ATOM	2461	OH2 TIP S 2			-10.821	1.00 37.31	s
	ATOM ATOM	2462 2463	OH2 TIP S 2				1.00 38.12	s
	MOTA	2463	OH2 TIP S 2			37.881	1.00 46.29	S
	ATOM	2465	OH2 TIP S 2			-8.575	1.00 43.71	S
35	ATOM	2466	OH2 TIP S 2			7.246	1.00 41.43	S
33	ATOM	2467	OH2 TIP S 2				1.00 41.79	S
	ATOM	2468	OH2 TIP S 2			28.166	1.00 37.03	S
	ATOM	2469		91 37.095		26.442	1.00 45.08	S
	ATOM	2470	OH2 TIP S 2				1.00 48.60	S
40	ATOM	2471	OH2 TIP S 2		2.784	-7.841	1.00 41.89	S
	MOTA	2472	OH2 TIP S 2	98 36.447	45.321	18.644	1.00 54.91	S
	MOTA	2473	OH2 TIP S 2	99 49.029	23.328	1.767	1.00 30.55	S
	MOTA	2474	OH2 TIP'S 3	01 24.375	13.771	8.634	1.00 48.47	S
	MOTA	2475	OH2 TIP S 3	03 47.904	36.798	28.653	1.00 35.76	S
45	ATOM	2476	OH2 TIP S 3	05 51.156	40.821	27.172	1.00 43.59	S
	MOTA	2477	OH2 TIP S 3		28.917	35.227	1.00 42.60	S
	ATOM	2478	OH2 TIP S 3	07 58.462	28.373	6.251	1.00 46.15	S
	ATOM	2479	OH2 TIP S 3	08 41.964	30.940	36.712	1.00 48.26	S
	ATOM	2480	OH2 TIP S 3	13 51.176	-1.922	3.336	1.00 50.61	s
50	MOTA	2481	OH2 TIP S10		36.868	23.805	1.00 36.97	S
	ATOM	2482	OH2 TIP S10				1.00 44.40	s
	ATOM	2483	OH2 TIP S10				1.00 45.49	S
	MOTA	12484	OH2 TIP S10				1.00 24.43	S
	ATOM	2485	OH2 TIP S10				1.00 35.97	S
55	ATOM	2486	OH2 TIP S10				1.00 43.15	s s
	MOTA	2487	OH2 TIP S10				1.00 49.45	S
	MOTA	2488	OH2 TIP S10					S
	ATOM	2489	OH2 TIP S10				1.00 50.10 1.00 49.47	S
	ATOM	2490	OH2 TIP S10	12 32.479	2.978	14.158	1.00 43.4/	3

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	MOTA	2491	012	GLC	G	ı	48.557	11.372	-12.279	1.00 40.72	G
	ATOM	2492	C11	GLC	G	1	48.836	12.133	-11.097	1.00 38.05	Ģ
	MOTA	2493	C13	GLC	G	1	49.266	13.554	-11.476	1.00 38.09	G
	MOTA	2494	014	GLC	G	1	49.559	14.299	-10.292	1.00 33.99	G
5	MOTA	2495	C15	GLC	G	1	48.150	14.257	-12.257	1.00 37.32	G
	MOTA	2496	016	GLC	G	1	48.574	15.582	-12.604	1.00 36.74	G
	MOTA	2497	012	GLC	G	2	40.114	-6.634	-6.562	1.00 33.52	G
	MOTA	2498	C11	GLC	G	2	38.967	-6.592	-7.404	1.00 31.05	G
	MOTA	2499	C13	GLC	\mathbf{G}	2	37.712	-6.417	-6.552	1.00 31.56	G
10	MOTA	2500	014	GLC	G	2	36.554	-6.406	-7.389	1.00 30.70	G
	ATOM	2501	C15	GLC	G	2	37.792	-5.109	-5.761	1.00 30.03	G
	MOTA	2502	016	GĻC	G	2	36.609	-4.961	-4.975	1.00 29.66	G
	MOTA	2503	012	GLC	G	3	44.030	8.243	-13.470	1.00 37.90	G
	MOTA.	2504	C11	GLC	G	3	43.950	9.648	-13.690	1.00 38.47	G
15.	MOTA	2505	C13	GLC	G	3	42.747	•	-14.579	1.00 39.52	G
	MOTA	2506	014	GLC	G	3	41.551	9.526	-13.942	1.00 39.39	G
	MOTA	2507		GLC		3	42.878		-15.934	1.00 41.43	G
	MOTA	2508	016	GLC	G	3	41.736	9.613	-16.731	1.00 40.78	G
	MOTA	2509	012	GLC	G	. 5	40.556	1.005	2.289	1.00 45.25	G
20	MOTA	2510		GLC		5	40.966	2.332	1.960	1.00 40.56	G
	MOTA	2511	C13	GLC	G	5	40.187	3.327	2.814	1.00 40.36	G
	MOTA	2512	014	GLC	G	5	38.791	3.169	2.572	1.00 40.71	G
	MOTA	2513	C15	GLC	G	5	40.619	4.751	2.464	1.00 40.04	G
	ATOM	2514	016	GLC	G	5	39.885	5.681	3.256	1.00 36.89 _,	G
25	MOTA	2515	012	GLC	G	6	36.951	22.702	40.046	1.00 63.04	G
÷	MOTA	2516		GLC		6	37.592	21.583	39.422	1.00 62.46	G
	MOTA	2517	C13	GLC	G	6	38.104	21.978	38.030	1.00 61.14	G
	MOTA	2518	014	GLC	G	6	39.034	23.054	38.168	1.00 61.72	G
	MOTA	2519	C15	GLC	Ģ	6	36.948	22.429	37.126	1.00 60.51	G
30	MOTA	2520	016	GLC	G	6	35.992	21.372	36.960	1.00 58.61	G
	ATOM	2521		GLC		7	37.316	0.281	14.299	1.00 73.45	G
	MOTA	2522		GLC		7	37.655	-0.758	15.222	1.00 72.78	G
	ATOM	2523		GLC		7	36.592	-1.856	15.157	1.00 72.98	G
•	MOTA	2524		GLC		7	35.320	-1.299	15.498	1.00 73.88	G
35	ATOM	2525		GLC		7	36.924	-2.989	16.134	1.00 73.66	G
	MOTA	2526		GLC		7	36.972	-2.493	17.478	1.00 75.38	G
	MOTA	2527		GLC		8	51.921	21.898	5.908	1.00 62.51	G
	MOTA	2528				8	52.447	20.871	5.063	1.00 63.42	G
	MOTA	2529	•	GLC		8	51.476	20.597	3.908	1.00 64.28	G
40	MOTA	2530		GLC		8	51.297	21.794	3.150	1.00 66.28	G G
	MOTA	2531		GLC		8	50.121	20.137	4.448	1.00 64.49	G
	ATOM	2532		GLC		8	49.233	19.886	3.357	1.00 64.01	G
	ATOM	2533		GLC		10	36.044	3.7.499	29.523	1.00 56.89 1.00 56.97	G
45	ATOM	2534		GLC		10	35.164	36.645	30.259		
45	ATOM	2535		GLC		10	33.849	36.489	29.494 29.308	1.00 56.11 1.00 56.44	G
	MOTA	2536		GLC		10	33.248	37.772		1.00 55.84	G
	MOTA	2537		GLC		10	32.900	35.580	30.277 29.557	1.00 55.84	G
	MOTA	2538		GLC		10	31.674	35.442			N
	ATOM	2539		ATP		1	46.280	25.658	5.170	1.00 51.49 1.00 52.22	N
50	MOTA	2540	PG	ATP		1.	46.464	25.053	3.691	1.00 52.22	N
	ATOM	2541		ATP		1	47.406	23.911		1.00 51.41	N
	ATOM	2542		ATP		1	46.794	26.182			N
	ATOM	2543		ATP		1	44.976	24.513		1.00 51.01	N
	ATOM	2544	PB	ATP		1 1	44.560	22.969 22.898		1.00 50.20	N
55	ATOM	2545		ATP		1	43.083 45.345	22.890		1.00 49.41	N
	ATOM	2546		ATP		1	45.345	22.474		1.00 47.77	N
	ATOM	2547		ATP		1	45.075	20.613		1.00 47.77	N
	ATOM	2548	PA O10	ATP			45.547	20.013		1.00 43.81	N
	ATOM	2549	OTA	MIP	14		43.34/	20.271	0.754	1.00 45.01	-•

	ATOM	2550	O2A	ATP	N	1	45.807	20.035	3.270	1.00 45.03	N
	MOTA	2551	05*	ATP	N	1	43.516	20.223	2.245	1.00 41.73	N
	ATOM	2552	C5*	ATP	N	1	42.528	20.925	1.489	1.00 37.57	N
	ATOM	2553	C4*	ATP	N	1	41.127	20.379	1.776	1.00 39.45	N
5	ATOM	2554	04*	ATP	N	1	40.907	19.024	1.279	1.00 37.72	N
_	ATOM	2555		ATP		1	40.777	20.321	3.251	1.00 38.48	N.
	ATOM	2556		ATP	-	1	40.360	21.615	3.697	1.00 40.42	N
	ATOM	2557		ATP		ī	39.608	19.374	3.270	1.00 37.58	N
	ATOM	2558		ATP		1	38.410	20.076	2.924	1.00 35.98	N
10	ATOM	2559		ATP		1	39.939	18.346	2.173	1.00 35.55	Ŋ
	ATOM	2560	N9	ATP		î	40.628	17.156	2.747	1.00 31.76	N
	ATOM	2561	C8	ATP		1	41.864	17.126	3.274	1.00 30.49	N
		2562	N7	ATP		1	42.143	15.877	3.667	1.00 29.75	N
	ATOM		C5	ATP		1	41.088	15.118	3.390	1.00 27.49	N
1.5	ATOM	2563						15.116	2.810	1.00 27.43	N
15	ATOM	2564	C4	ATP		1	40.125		2.431	1.00 30.02	N
	ATOM	2565	N3	ATP		1	38.937	15.389		1.00 27.11	N
	ATOM	2566	C2	ATP		1	38.679	14.085	2.615 3.175	1.00 23.62	N
	ATOM	2567	N1	ATP		1	39.597	13.283		1.00 21.76	N
00	ATOM	2568	C6	ATP		1	40.800		3.571		N
20	MOTA	2569	N6	ATP		1	41.698	12.964	4.127	1.00 21.94	I
	MOTA	2570	S	SO4		1	58.680	8.493	-0.639	1.00 56.05	
	ATOM	2571	01	S04		1	57.956	7.875	0.483	1.00 58.83	I
	MOTA	2572	02	S04		1	57.886	9.607	-1.188	1.00 57.04	I
~-	MOTA	2573	03	SO4		1	58.906	7.478	-1.683	1.00 57.47	I
25	MOTA	2574	04	S04		1	59.976	9.008	-0.156	1.00 57.51	I
	MOTA	2575	s	SO4		2	39.339	4.855	7.057	1.00 84.24	ī
	ATOM	2576	01	S04		2	39.390	6.175	7.711	1.00 85.02	ī
	ATOM	2577	02	SO4		2	40.101	4.897	5.797	1.00 84.75	I
	ATOM	2578	03	S04		2	37.936	4.506	6.766	1.00 84.94	I
30	MOTA	2579	04	S04		2	39.931	3.842	7.954	1.00 84.44	I
	- ATOM	2580	S	SO4		3	38.987	-2.256	3.310	1.00 58.58	I
	ATOM	2581	01	504		3	37.734	-1.675	3.827	1.00 59.11	I
	MOTA	2582	02	SO4		3	39.460	-1.454	2.172	1.00 59.91	I
	MOTA	2583	03	SO4	I	3	38.743	-3.640		1.00 60.97	I
35	ATOM	2584	04	SO4	I	3	40.014	-2.260	4.369	1.00 59.58	I
	ATOM	2585	S	SO4		4	34.397	5.289	30.981	1.00 64.34	I
	MOTA	2586	01	SO4	I	4	33.627	6.528	30.742	1.00 60.43	I
	ATOM	2587	02	SO4		4	34.337	4.427	29.782	1.00 60.11	· I
	ATOM	2588	03	SO4	I	4	33.816	4.572	32.133	1.00 64.39	Ī
40	ATOM	2589	04	SO4		4	35.806	5.626	31.277	1.00 63.55	I
	ATOM	2590	S	SO4	Ι	5	55.074	-6.984	-3.711	1.00 75.40	I
	ATOM	2591	01	SO4	I	5	54.657	-7.518	-2.399	1.00 74.66	I
	ATOM	2592	02	SO4	Ί	5	54.209	-5.845	-4.065	1.00 74.96	I
	MOTA	2593	03	SO4	I	5	54.950	-8.034	-4.742	1.00 74.22	I
45	MOTA	2594	04	SO4	Ι	5	56.477	-6.532	-3.633	1.00 75.15	I
	ATOM	2595	02	PO4	P	100	57.362	24.998	13.149	1.00 66.76	P
	ATOM	2596	03	PO4	P	100	59.399	26.166	13.761	1.00 66.89	P
	ATOM	2597	04	PO4	P	100	57.761	25.606	15.462	1.00 67.43	P
	MOTA	2598	01	PO4	P	100	57.264	27.325	13.818	1.00 65.91	P
50	ATOM	2599	P	PO4	P	100	57.947	26.025	14.048	1.00 66.69	P
	MOTA	2600	CB	GLU		80	50.411	3.975	-13.538	0.50 23.31	AC2
	ATOM	2601	CG	GLU		80	51.306	4.896	-14.362	0.50 24.09	AC2
	ATOM	2602	CD	GLU		80	52.180	5.798	-13.509	0.50 25.31	· AC2
	ATOM	2603	OE1	GLU		80	52.841	5.289	-12.580	0.50 22.80	AC2
55·	MOTA	2604	OE2	GLU		80	52.212	7.018	-13.774	0.50 28.07	AC2
	ATOM	2605	CB	SER		105	37.582	-1.281	-6.192	0.50 21.16	AC2
	ATOM	2606	OG	SER		105	37.127	-1.871	-4.988	0.50 20.42	AC2
	ATOM	2607	CB	ARG		116	59.520	22.977	-7.867	0.50 31.00	AC2
	ATOM	2608	CG	ARG		116	60.312	24.192	-8.323	0.50 32.50	AC2

114

	MOTA	2609	CD	ARG	116	60.266	24.349	-9.838	0.50 34.11	AC2
	ATOM	2610	NE	ARG	116	61.045	25.499	-10.290	0.50 36.67	AC2
	ATOM	2611	CZ	ARG	116	60.729	26.766	-10.035	0.50 37.26	AC2
	ATOM	2612	NH1	ARG	116	59.642	27.053	-9.331	0.50 38.99	AC2
5	ATOM	2613	NH2	ARG	116	61.503	27.746	~10.479	0.50 37.83	AC2
	ATOM	2614	CB	LEU	145	49.693	8.642	6.631	0.50 15.29	AC2
	ATOM	2615	CG	LEU	145	50.783	8.664	5.552	0.50 14.29	AC2
	ATOM	2616	CD1	LEU	145	50.264	9.373	4.305	0.50 8.20	AC2
	ATOM	2617	CD2	LEU	145	52.030	9.361	6.087	0.50 10.66	AC2
10	ATOM	2618	CB	ARG	183	27.455	16.155	24.989	0.50 19.21	AC2
	MOTA	2619	. CG	ARG	183	28.077	15.397	26.147	0.50 18.46	AC2
	ATOM	2620	CD	ARG	183	27.002	14.945	27.127	0.50 19.72	AC2
	ATOM	2621	NE	ARG	183	26.016	14.086	26.478	0.50 18.79	AC2
	ATOM	2622	cz	ARG	183	24.703	14.279	26.539	0.50 18.52	AC2
15	ATOM	2623	NHl	ARG	183	24.213	15.305	27.221	0.50 15.35	AC2
	ATOM	2624	NH2	ARG	183	23.881	13.445	25.915	0.50 17.55	AC2
	ATOM	2625	CB	SER	191	38.479	10.847	23.036	0.50 16.57	AC2
	ATOM	2626	OG	SER	191	37.418	10.765	23.973	0.50 18.62	AC2
	ATOM	2627	CB	GLU	209	38.645	24.079	8.551	0.50 22.02	AC2
20	ATOM	2628	CG	GLU	209	37.769	25.296	8.263	0.50 23.40	AC2
	ATOM	2629	CD	GLU	209	37.513	26.175	9.483	0.50 24.27	AC2
	MOTA	2630	OE1	GLU	209	37.076	27:328	9.288	0.50 25.25	AC2
	ATOM	2631	OE2	GLU	209	37.737	25.727	10.629	0.50 20.24	AC2
	ATOM	2632	CB	GLN	247	38.598	32.546	14.790	0.50 18.71	AC2
25	ATOM	2633	CG	GLN	247	38.077	33.665	13.900	0.50 16.95	AC2
	ATOM	2634	CD	GLN	247	38.614	33.598	12.479	0.50 19.13	AC2
	ATOM	2635	OE1	GLN	247	39.763	33.221	12.246	0.50 17.24	AC2
	ATOM	2636	NE2	GLN	247	37.780	33.979	11.520	0.50 19.88	AC2
	MOTA	2637	CE	LYS	315	34.978	25.150	36.369	0.50 20.49	AC2
30	MOTA	2638	NZ	LYS	315	34.183	24.074	37.023	0.50 17.05	AC2
	MOTA	2639	CB	GLN	352	32.365	1.170	19.731	0.50 31.10	AC2
	MOTA	2640	CG	ĞЃИ	352	33.833	0.778	19.683	0.50 32.11	AC2
	ATOM	2641	$^{\rm CD}$	GĽN	352	, 34.190	0.027	18.419	0.50 33.04	AC2
	ATOM	2642	OE1	GLN	352	33.906	0.485	17.314	0.50 34.87	AC2
35	ATOM	2643	NE2	GLN	352	34.819	-1.133	18.575	0.50 32.08	AC2
	END									

Example 3: Co-ordinates for the PDK1 fragment without alternate side chains.

```
40
    REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free_r= 0.2220
                  r= 0.1954 free r= 0.2224
    REMARK final
    REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0
    REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
    REMARK rweight= 0.0900 (with wa= 1.29263)
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1 : /dd1/david/projects/PDK1_new/CNS/prot.par
    REMARK parameter file 2 : /ddl/david/projects/PDK1_new/CNS/atp.par
    REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
    REMARK parameter file 4 : CNS_TOPPAR:ion.param
```

```
REMARK parameter file 5 : /dd1/david/projects/PDK1_new/CNS/glycerol.par
    REMARK molecular structure file: ../generate/alternate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../1/hkl/cns.hkl
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.0
    REMARK initial B-factor correction applied to fobs :
             B11= -2.766 B22= -2.766 B33=
                                               5.532
    REMARK
             B12= -0.375 B13=
    REMARK
                                 0.000 B23=
                                                0.000
    REMARK B-factor correction applied to coordinate array B:
10
    REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
    REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range:
                                                                    28210 ( 100.0
15
    REMARK number of unobserved reflections (no entry or |F|=0):
                                                                      568 (
     용 )
    REMARK number of reflections rejected:
                                                                         0 (
                                                                               0.0
    REMARK total number of reflections used:
                                                                     27642 (
                                                                              98.0
20.
     ୫ )
                                                                              95.9
    REMARK number of reflections in working set:
                                                                     27063 (
                                                                       579 (
    REMARK number of reflections in test set:
                                                                               2.1
25
    ቄ )
                                47.624 90.00 90.00 120.00 P 32 2 1
     CRYST1 123.013 123.013
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE:16-Apr-2002 18:31:12
                                              created by user: david
    REMARK VERSION:1.0
                                                       8.216 1.00 67.78
30
    ATOM
               1 CB PRO A
                             71
                                      58.912
                                              -7.251
    MOTA
                      PRO A
                             71
                                      59.621
                                             -6.941
                                                       9.534 1.00 69.16
                                                                               Α
               2 CG
                                      59.493
                                              -6.506
                                                       5.894
                                                              1.00 67.06
                                                                               Ά
    ATOM
               3
                 С
                      PRO A
                             71
                                      59.196
                                              -5.318
                                                       5.766
                                                              1.00 66.66
                                                                               Α
                 0
                      PRO A
                             71
    MOTA
               4
    ATOM
               5
                 N
                      PRO A
                             71
                                      60.984
                                              -6.073
                                                       7.833
                                                              1.00 67.86
                                                                               Α
35
                                      60.554
                                              -5.762
                                                       9.207
                                                              1.00 68.24
    MOTA
               6
                  CD
                      PRO A
                             71
    MOTA
               7
                  CA
                      PRO A
                             71
                                      60.040
                                              -7.035
                                                       7.217
                                                              1.00 67.75
                                                                               Α
                                              -7.385
                                      59.356
                                                       4.890
                                                              1.00 66.32
                                                                               Α
    ATOM
               8
                  N
                      PRO A
                             72
                  CD
                      PRO A
                             72
                                      59.712
                                              -8.816
                                                       4.898
                                                              1.00 67.17
                                                                               Α
    ATOM
               9
              10
                  CA
                      PRO A
                             72
                                      58.840
                                              -6.986
                                                       3.578
                                                              1.00 65.61
    ATOM
40
                  CB
                      PRO A
                                      58.672
                                              -8.321
                                                       2.858
                                                              1.00 66.47
                                                                               Α
    MOTA
              11
                             72
                      PRO A
                                      59.796
                                              -9.133
                                                       3.419
                                                              1.00 67.57
                                                                               A
    MOTA
              12
                  CG
                             72
              13
                      PRO A
                                              -6.208
                                                              1.00 63.94
                                                                               Α
                 C
                             72
                                      57.527
                                                       3.673
    MOTA
                 ÷o
    ATOM
              14
                      PRO A
                             72
                                      56.710
                                              -6.451
                                                       4.561
                                                              1.00 64.11
                                                                               Α
    MOTA
              15
                  N
                      ALA A
                             73
                                      57.341
                                              -5.268
                                                       2.753
                                                              1.00 61.57
                                                              1.00 58.74
45
    ATOM
              16
                  CA
                      ALA A
                             73
                                      56.133
                                              -4.454
                                                       2.708
                                                                               Α
                                                              1.00 58.05
                                              -3.030
                                                                               Α
                  CB
                      ALA A
                             73
                                      56.438
                                                       3.165
    ATOM
              17
                  C
                      ALA A
                             73
                                      55.626
                                              -4.448
                                                       1.271
                                                              1.00 56.78
    MOTA
              18
              19
                  0
                      ALA A
                             73
                                      56.347
                                              -4.834
                                                       0.349
                                                              1.00 56.95
    ATOM
                  N
                      PRO A
                                      54.372
                                              -4.024
                                                       1.057
                                                              1.00 54.15
                                                                               Α
    ATOM
              20
                             74
50
     MOTA
              21
                  CD
                      PRO A
                             74
                                      53.335
                                              -3.610
                                                       2.018 1.00 53.31
                                                                               Α
                                              -4.003
                      PRO A
                                      53.856
                                                                               Α
                  CA
                                                      -0.314
                                                              1.00 52.54
    ATOM
              22
                             74
                  CB
                      PRO A
                             74
                                      52.474
                                              -3.375
                                                      -0.148
                                                              1.00 52.86
                                                                               Α
    ATOM
              23
     MOTA
              24
                  CG
                      PRO A
                             74
                                      52.067
                                              -3.824
                                                       1.226 .1.00 52.88
                                                                               Α
                                                              1.00 50.08
                                              -3.167
                                                                               А
     ATOM
              25
                  С
                      PRO A
                             74
                                      54.772
                                                      -1.204
                                                              1.00 49.96
                                                                               Α
55
              26
                  0
                      PRO A
                             74
                                      55.559
                                              -2.361
                                                      -0.708
     ATOM
    ATOM
              27
                 N
                      ALA A
                             75
                                      54.680
                                              -3.366
                                                      -2.514
                                                              1.00 47.58
                  CA
                      ALA A
                             75
                                      55.503
                                              -2.602
                                                              1.00 44.69
                                                                               A
     MOTA
              28
                                                      -3.446
                                                                               Α
              29
                  CB
                      ALA A
                             75
                                      55.312
                                              -3.121
                                                      -4.870
                                                              1.00 46.14
     MOTA
                  С
                      ALA A
                                                              1.00 41.55
     ATOM
              30
                             75
                                      55.100
                                              -1.134
                                                      -3.371
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											_
	ATOM	31	0	ALA	Α	75	53.947	-0.813	-3.086	1.00 41.01	A
	ATOM	32	N	LYS	Α	76	56.053	-0.245	-3.619	1.00 38.31	A
	ATOM	33	CA	LYS	Α	76	55.781	1.184	-3.588	1.00 35.72	A
	ATOM	34	CB	LYS	A	76	57.053	1.957	-3.930	1.00 37.70	A
5	ATOM	35	CG	LYS	A	76	57.123	3.356	-3.350	1.00 40.99	Α
•	ATOM	36	CD	LYS	Α	76	57.262	3.316	-1.836	1.00 40.04	A
	ATOM	37	CE	LYS		76	57.511	4.705	-1.277	1.00 42.08	A
	ATOM	38	NZ	LYS		76	57.681	4.695	0.202	1.00 42.99	A
	ATOM	39	C	LYS		76	54.708	1.467	-4.638	1.00 32.65	A
10	ATOM	40	o	LYS		76	54.814	1.005	-5.770	1.00 31.41	A
10				LYS		77	53.668	2.207	-4.270	1.00 28.59	A
	ATOM	41	N				52.619	2.517	-5.232	1.00 25.72	A
	MOTA	42	CA	LYS		77		2.865	-4.509	1.00 26.22	A
	ATOM	43	CB	LYS		77	51.316		-3.631	1.00 20.22	A
	MOTA	44	CG	LYS		77	50.796	1.731		1.00 27.13	A
15	ATOM	45	CD	LYS		77	49.487	2.089	-2.967		
	MOTA	46	CE	LYS		77	49.136	1.091	-1.870	1.00 27.31	A
	MOTA	47	NZ	LYS	Α	77	48.998	-0.296	-2.380	1.00 27.17	A
	MOTA	48	C	LYS	A	77	53.053	3.668	-6.137	1.00 24.67	A
	ATOM	49	0	LYS	Α	77	54.010	4.377	-5.829	1.00 21.60	A
20	MOTA	50	N	ARG	A	78	52.351	3.838	-7.254	1.00 23.66	A
	MOTA	51	CA	ARG	Α	78	52.662	4.897	-8.211	1.00 26.14	Α
	ATOM	52	CB	ARG	А	78	53.574	4.344	-9.318	1.00 28.57	A
	MOTA	53	CG	ARG	Α	78	53.017	3.139	-10.050	1.00 34.78	A
	ATOM	54	CD	ARG	А	78	54.092	2.465	-10.896	1.00 40.96	Α
25	ATOM	55	NE	ARG	Α	78	53.560	1.364	-11.700	1.00 48.93	A
	ATOM	56	CZ	ARG		78		0.270	-11.203	1.00 52.58	A
	ATOM	57		ARG		78	52.860	0.113	-9.889	1.00 54.60	A
	ATOM	58		ARG		78	52.530		-12.022	1.00 54.09	A
	ATOM	59	C	ARG		78	51.382	5.488	-8.803	1.00 23.76	A
20			0	ARG		78	50.311	4.888	-8.706	1.00 24.25	A
30	ATOM	60		PRO		79	51.475	6.676	-9.428	1.00 21.76	A
	ATOM	61	N				52.691	7.475	-9.668	1.00 20.82	A
	MOTA	62	CD	PRO		79 70	50.301		-10.021	1.00 21.96	A
	MOTA	63	CA	PRO		79				1.00 21.30	A
	MOTA	64	CB	PRO		79	50.910		-10.816	1.00 22.27	A
35	MOTA	65	CG	PRO		79	52.124		-10.014		A
	ATOM	66	C	PRO		79	49.446		-10.903	1.00 22.86	
	ATOM	67	0	PRO		79	48.213		-10.842	1.00 20.52	A
	MOTA	68	N	GLU		80	50.103		-11.714	1.00 21.87	A
	MOTA	69	CA	GLU	А	80	49.403		-12.628	1.00 22.99	A
40	MOTA	70	CB	GLU	Α	80	50.393		-13.571	1.00 25.24	Α
	MOTA	71	CG	GLU	A	80	51.230		-12.925	1.00 28.75	A
	ATOM	72	CD	GLU	Α	80	52.157	2.224	-13.913	1.00 31.99	A
	MOTA	73	OE1	GLU	A	80	53.072	2.897	-14.433	1.00 34.34	A
	ATOM	74	OE2	GLU	A	80	51.969		-14.172	1.00 32.83	A
45	ATOM	75	C	GLU	Α	80	48.556	3.631	-11.912	1.00 22.09	A
	MOTA	76	0	GLU	Α	80	47.692	3.013	-12.530	1.00 22.37	A
	ATOM	77	N	ASP	A	81	48.804	3.413	-10.622	1.00 19.97	A
	ATOM	78	CA	ASP	Α	81	48.026	2.423	-9.874	1.00 19.93	A
	ATOM	79	CB	ASP		81	48.736	2.029	-8.571	1.00 21.19	A
50	ATOM	80	ĊĠ	ASP		81	50.089	1.380	-8.807	1.00 22.46	A
50	ATOM	81		ASP		81	50.195	0.554	-9.731	1.00 24.22	Α
	ATOM	82		ASP		81	51.043	1.685	-8.058	1.00 23.33	A
		83	C	ASP		81	46.652	2.975	-9.518	1.00 20.85	A
	ATOM			ASP		81	45.793	2.246	-9.015	1.00 19.96	A
- م	ATOM	84						4.258	-9.804	1.00 18.91	A
55	ATOM	85	N	PHE		82	46.445			1.00 10.31	A
	ATOM	86	CA	PHE		82	45.200	4.934	-9.465	1.00 13.30	A
	MOTA	87	CB	PHE		82	45.475	6.027	-8.427	1.00 18.43	A
	MOTA	88	CG	PHE		82	46.134	5.531	-7.175	1.00 18.01	A
	MOTA	89	CD1	PHE	Α	82	45.371	5.136	-6.084	1.00 17.19	ų

	MOTA	90	CD2	PHE	Α	82	-	47.520	5.460	-7.086	1.00	18.99	A
	MOTA	. 91		PHE		82		45.977	4.676	-4.918	1.00		Α
	MOTA	92	CE2	PHE	Α	82		48.137	5.000	-5.925	1.00		A
	MOTA	93	CZ	PHE	Α	82		47.361	4.607	-4.838	1.00		A
5	MOTA	94	C	PHE	Α	82		44.476		-10.621	1.00		A
	MOTA	95	0	PHE	A	82		45.066		-11.649	1.00		A
	MOTA	96	N	LYS	Α	83		43.182		-10.411	1.00		A
	MOTA	97	CA	LYS	Α	83		42.321		-11.353	1.00		A
	ATOM	98	CB	LYS		83		41.096		-11.687	1.00		A
10	MOTA	99	CG	LYS		83		40.062		-12.550	1.00		A
	MOTA	100	CD	LYS		83		38.974		-12.981	1.00		A
	MOTA	101	CE	LYS		83		37.909		-13.824	1.00		A
	MOTA	102	NZ	LYS		83		37.179		-13.043	1.00		A
	MOTA	103	С	LYS		83		41.913		-10.541		20.74	A
15	MOTA	104	0	LYS		83		41.084	7.606	-9.635		20.98	. A
	MOTA	105	И	PHE		84		42.513		-10.835		19.99	A
	MOTA	106	CA	PHE		84		42.188		-10.083		18.63	A
	MOTA	107	CB	PHE		84		43.279		-10.258		18.95	Α
	MOTA	108	CG	PHE		84	•	44.571	10.741	-9.587		17.68	A
20	ATOM	109		PHE		84		45.498		-10.224		18.16	A
	ATOM	110		PHE		84		44.843	11.183	-8.299		19.66	A
	ATOM	111		PHE		84		46.676	9.556	-9.589		18.09	A
	ATOM	112		PHE		84		46.021	10.816	-7.653		18.89	A
	MOTA	113	CZ	PHE		84		46.936	10.002	-8.301		17.33	A A
25	MOTA	114	C	PHE		84		40.834		-10.460		19.69 20.72	A
	ATOM	115	0	PHE		84		40.391		-11.601		16.80	A
	MOTA	116	N	GLY		85		40.178	11.233	-9.484		17.73	A
	ATOM	117	CA	GLY		85		38.872	11.810	-9.716		18.75	A
••	MOTA	118	C	GLY		85		38.819	13.280	-9.346 -9.650		18.45	A
30	ATOM	119	0	GLY		85		39.740	14:043	-8.659		16.00	A
	MOTA	120	И	LYS		86		37.753	13.673 15.064	-8.278	-	18.26	A
	ATOM	121	CA	LYS		86		37.571	15.302	-7.812		19.00	A
	ATOM	122	CB	LYS		86		36.133 35.793	14.660	-6.481		21.55	A
35	ATOM	123 124	CD	LYS LYS		86 86		34.368	14.981	-6.066		26.48	A
33	ATOM ATOM	125	CE	LYS		86		33.994	14.239	-4.793		31.92	A
	ATOM	126	NZ	LYS		86		32.568	14.457	-4.412		35.36	A.
	ATOM	127	C	LYS		86		38.523	15.571	-7.202		18.57	A
	MOTA	128	0	LYS		86		39.045	14.807	-6.385		16.77	A
40	MOTA	129	N	ILE		87		38.737	16.881	-7.227		17.88	A
40	ATOM	130	CA	ILE		87		39.577	17.554			18.26	A
	MOTA	131	CB	ILE		87		39.994	18.952	-6.772		19.60	A
	ATOM	132	CG2			87		40.593	19.786		1.00	18.73	A
	ATOM	133		ILE		87		40.968	18.786		1.00	21.16	A
45	ATOM	134		ILE		87		41.412	20.087		1.00	25.26	Α
	ATOM	135	C	ILE		87		38.731	17.709			19.67	A
•	ATOM	136	0	ILE		87		37.628	18.249		1.00	20.41	A
	ATOM	137	N	LEU		88		39.240	17.229	-3.867	1.00	19.15	A
	ATOM	138	CA	LEU		88		38.508	17.324	-2.611	1.00	20.68	A
50	ATOM	139	CB	LEU		88		38.870	16.151	-1.700	1.00	19.97	Α
	ATOM	140	CG	LEU		88		38.529	14.759	-2.237	1.00	19.24	A
	ATOM	141		LEU		88		39.090	13.692	-1.311		21.41	A,
	ATOM	142	CD2	LEU	Α	88		37.029	14.622	-2.359		18.84	A
	MOTA	143	C	LEU	Α	88		38.815	18.632			23.11	A ·
55	MOTA	144	0	LEU	Α	88		37.999	19.146			25.10	A
	MOTA	145	N	GLY		89		39.997	19.174			24.09	A
	MOTA	146	CA	GLY		89		40.367	20.418			24.27	· A
	MOTA	147	C	GLY	Α	89		41.658	20.954			25.47	A
	МОТА	148	0	GLY	· A	89		42.445	20.202	-2.666	1.00	22.19	A

	MOTA	149	N	GLU	Α	90	41.8	370	22.254	-1.906	1.00	26.22	A
	ATOM	150	CA	GLU		90	43.0	064	22.924	-2.404	1.00	29.96	A
	MOTA	151	CB	GLU	Α	90	42.6	598	23.814	-3.596	1.00	30.75	A
	ATOM	152	CG	GLU	Α	90	42.2	267	23.038	-4.831	1.00	34.32	A
5	ATOM	153	CD	GLU		90	41.7	711	23.930	-5.927	1.00	38.27	A
-	ATOM	154		GLU		90	40.5	590	24.456	-5.764	1.00	40.57	A
	ATOM	155		GLU		90	42.3	398	24.110	-6.952	1.00	40.90	· A
	MOTA	156	C	GLU		90	.43.7	711	23.768	-1.313	1.00	30.68	A
	ATOM	157	ō	GLU		90	43.0	149	24.574	-0.668	1.00	32.83	A
10	ATOM	158	N	GLY		91	45.0	006	23.566	-1.104	1.00	29.66	A
	ATOM	159	CA	GLY		91	45.7	724	24.332	-0.104	1.00	29.40	A
	ATOM	160	C	GLY		91 .	46.7	795	25.151	-0.798	1.00	29.98	A
	ATOM	161	ō	GLY		91			25.130	-2.028	1.00	28.16	A
	ATOM	162	N	SER		92	47.6	505	25.870	-0.029	1.00	28.30	A
15	MOTA	163	CA	SER		92	48.6		26.681	-0.633	1.00	30.50	A
1,5	ATOM	164	СВ	SER		92	49.		27.717	0.370	1.00	32.43	A
	ATOM	165.	OG	SER		92	49.5		27.099	1.593	1.00	40.94	A
	ATOM	166	C	SER		92	49.8		25.843	-1.164	1.00	29.77	Α
	ATOM	167	Ö	SER		92	50.4		26.221	-2.143	1.00	30.46	A
20		168	N	PHE		93	50.0		24.703	-0.536	1.00	27.65	A
20	MOTA MOTA	169	CA	PHE		93	51.		23.855	-0.995		26.34	A
		170	CB	PHE		93	52.3		23.785	0.068		27.95	A
	ATOM	171	CG	PHE		93	52.		25.117			31.06	A
	ATOM			PHE		93	52.		25.909	1.392		29.96	A
25	ATOM	172 173		PHE		93	53.		25.613	-0.308		31.38	A
23	ATOM			PHE		93	52.		27.181	1.665		32.69	A
	ATOM	174		PHE			54.		26.883	-0.044		32.63	A
	MOTA	175	CEZ	PHE		93	53.		27.670	0.945		31.81	A
	ATOM	176	C	PHE		93	50.		22.445	-1.365		25.39	A
20	MOTA	177				93	51.		21.559	-1.522		24.59	A
30	MOTA	178	0	PHE		94	49.		22.235	-1.519		23.63	A `
	MOTA	179	N	SER		94	48.		20.912	-1.860		21.43	A
	MOTA	180	CA	SER		94	49.		20.013	-0.628		21.42	A
	MOTA	181	CB	SER			48.		20.475	0.340		21.19	A
26	ATOM	182	OG	SER		94		539	20.925	-2.378		19.82	A
35	ATOM	183	C	SER		94		795	21.882	-2.173		18.76	A
	ATOM	184	0	SER		94		174	19.832	-3.038		19.38	· A
	ATOM	185	N	THR		95		840	19.637	-3.580		17.98	A
	ATOM	186	CA	THR		95			19.818	-5.110		19.25	A
40	ATOM	187	CB	THR		95		818	21.162	-5.434		22.04	A
40	MOTA	188		THR		95.		196	19.549	-5.661		17.61	A
	MOTA	189		THR		95		421		-3.243		18.61	A
	MOTA	190	C	THR		95		455	18.201	-3.524		17.10	A
	ATOM	191	0	THR		95		212	17.264	-2.623		16.53	A
	ATOM	192	N	VAL		96		295	18.024	-2.266		16.05	A
45	ATOM	193	CA	VAL				845				16.32	A
	MOTA	194	CB	VAL				170	16.672	-0.886		18.02	A
	MOTA	195		LVAI				741	15.249	-0.532		16.69	A
	MOTA	196		VAI				145	17.206	0.168			A
	MOTA	197	С	VAI				875	16.207	-3.335		16.42 16.47	A
50	MOTA	198	0	VAI		96		906	16.892	-3.665			A
	MOTA	199	N	VAI				157	15.033	-3.888		16.80	A
	ATOM	200	CA	VAI				338	14.471	-4.949			A
	ATOM	201	CB	VAI		97		153	14.354	-6.255		18.43	A
	MOTA	202		L VAI				249	13.927	-7.404		19.69	A A
55	MOTA	203		IAV S				831	15.685	-6.569		17.84	A
	MOTA	204	C	IAV				812	13.091	-4.583		16.77	
	MOTA	205	0	IAV				532	12.270	-4.014		17.13	A A
	MOTA	206	N	LEU				545	12.845	-4.895	1.00	16.62	A
	ATOM	207	CA	LEU	JA	98	39.	947	11.548	-4.624	1.00	17.04	A

	ATOM	208	СВ	LEU	Α	98	3	8.424		11.633	-4.743	1.00	16.89	A
	MOTA	209	CG	LEU	A	98	3	7.635	;	10.342	-4.508		19.46	A
	ATOM	210	CD1	LEU	Α	98	3	7.990)	9.762	-3.146	1.00	20.07	A
	MOTA	211	CD2	LEU	Α	98	3	6.143		10.627	-4.588		17.93	A
5	ATOM	212	C	LEU	Α	98	4	0.512	:	10.597	-5.677		17.38	A
	ATOM	213	0	LEU	Α	98	4	0.527	,	10.920	-6.863	1.00	18.60	A
	ATOM	214	N	ALA	Α	99	4	0.995	5	9.438	-5.246	1.00	17.13	A
	ATOM	215	CA	ALA	Α	99	4	1.570)	8.466	-6.168	1.00	18.42	A
	ATOM	216	СВ	ALA	Α	99	4	3.090)	8.524	-6.105	1.00	14.76	A
10	ATOM	217	С	ALA	Α	99	. 4	1.102	2	7.055	-5.848	1.00	21.40	A
	ATOM	218	0	ALA	Α	99	4	0.941	L	6.691	-4.679	1.00	22.52	A
	MOTA	219	N	ARG	A	100	4	0.878	3	6.261	-6.888	1.00	19.77	A
	ATOM	220	CA	ARG	Α	100	4	0.459	•	4.884	-6.693	1.00	20.85	A
	ATOM	221	CB	ARG	Α	100	3	9.202	2	4.585	-7.518	1.00	24.22	Α
15	ATOM	222	CG	ARG	A	100	3	8.608	3	3.205	-7.256	1.00	31.78	A
	MOTA	223	CD	ARG	Α	100	3	7.326	5	2.979	-8.048	1.00	36.24	A
	MOTA	224	NE	ARG	Α	100	3	6.213	3	3.818	-7.594	1.00	41.40	A
	ATOM	225	CZ	ARG	A	100	3	5.566	5	3.662	-6.439	1.00	42.05	A
	ATOM	226	NH1	ARG	Α	100	3	5.912	2	2.696	-5.598	1.00	40.67	A
20	ATOM	227	NH2	ARG	Α	100	3	4.559	9	4.468	-6.128	1.00	43.65	A
-	ATOM	228	С	ARG	Α	100	4	1.613	3	3.985	~7.129	1.00	18.63	A
	ATOM	229	0	ARG	Α	100	4	2.078	3	4.065	-8.271	1.00	19.49	A
	ATOM	230	N	GLU	Α	101	4	2.102	2	3.157	-6.212	1.00	16.43	A
	ATOM	231	CA	GLU	Α	101	4	3.196	5	2.246	-6.533	1.00	16.11	A
25	ATOM	232	CB	GLU	Α	101	4	3.774	1	1.637	-5.248		16.79	A
	MOTA	233	CG	GLU	Α	101	4	4.917	7	0.657	-5.488		16.51	A
	MOTA	234	CD	GLU	A	101	4	5.501	1	0.115	-4.200		18.20	Ą
	ATOM	235	OE1	${\tt GLU}$	Α	101	4	4.733	3	-0.081	-3.239		18.32	. A
	MOTA	236	OE2	GLU	A	101	4	6.725	5	-0.132	-4.150		17.14	A
30	ATOM	237	C	GLU	Α	101	4	2.625	5	1.152	-7.442		17.92	A.
	MOTA	238	0	GLU	Α	101		1.683		0.462	-7.069		18.02	A
	ATOM	239	N	LEU	Α	102	4	3.198	8	1.002	-8.632		19.06	A
	MOTA	240	CA	LEU	Α	102	4	2.718	В	0.025	-9.607		20.71	A
	MOTA	241	CB	LEU	Α	102		3.569			-10.878		23.42	A
35	MOTA	242	CG			102		3.531			-11.642		25.30	A
	MOTA	243		LEU				4.577			-12.748		27.88	A .
	ATOM	244	CD2	LEU	Α	102		2.140			-12.214		26.79	A
	MOTA	245	C			102		2.67		-1.418	-9.125		21.62	A A
	ATOM	246	0			102		1.668		-2.103	-9.305		21.09	A A
40	MOTA	247	N			103		3.75		-1.874	-8.507		19.38	A
	MOTA	248	CA			103		13.836		-3.249	-8.035		20.87 19.23	A
*	ATOM	249	CB			103		5.284		-3.571	-7.671		19.23	A
	MOTA	250	C			103		2.91		-3.629	-6.872		20.38	A
	MOTA	251	0		-	103		2.70		-4.815	-6.628			_
45	MOTA	252	N		•	104		2.36		-2.643	-6.175		18.12 17.15	A A
	ATOM	253	CA			104		11.51		-2.927	-5.018		19.54	A
	ATOM	254	CB			104		2.21		-2.484			19.26	A
	ATOM	255		THR				12.45		-1.070	-3.773 -3.529		17.02	A
	MOTA	256		THR				13.53		-3.219			19.44	A
50	ATOM	257	C			104		10.15		-2.247	-5.026		18.70	A
	ATOM	258	0			104		39.25 10.03		-2.648 -1.207	-4.285 -5.847		19.65	A
	ATOM	259	N			105							19.37	A
	MOTA	260	CA			105		38.81:		-0.400			21.81	A
	ATOM	261	CB			105		37.59 36.43		-1.304 -0.539			23.01	A
55	ATOM	262	og			105		38.64		0.447			18.99	A
	ATOM	263	C			105		37.60		1.070			18.66	. A
	ATOM	264	O N			105		39.67		0.468			16.84	A
	ATOM	265	N			106		39.65		1.267			16.21	A
	MOTA	.266	CA	AKG	H	. 106		, , , , , ,	-	4.201	~.034		· · 	

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	MOTA	267	CB	ARG	Α	106		40.827	0.886	-1.723	1.00 16.41	A
	MOTA	268	CG	ARG	Α	106		40.619	-0.367	-0.906	1.00 15.49	A
	MOTA	269	CD	ARG	A	106		41.887	-0.755	-0.170	1.00 17.43	A
	MOTA	270	NE	ARG	Α	106		41.620	-1.792	0.824	1.00 20.47	A
5	MOTA	271	\mathbf{cz}	ARG	A	106		42.548	-2.568	1.371	1.00 20.24	A
	MOTA	272	NH1	ARG	Α	106		43.821	-2.433	1.017	1.00 17.80	A
	MOTA	273	NH2	ARG	A	106		42.198	-3.468	2.285	1.00 20.14	, A ,
	ATOM	274	С	ARG	A	106		39.785	2.746	-2.981	1.00 17.37	A
	MOTA	275	0	ARG				40.514	3.103	-3.902	1.00 17.75	A
10	MOTA	276	N			107		39.085	3.599	-2.240	1.00 16.06	, A
	MOTA	277	CA	GLU	A	107		39.156	5.039	-2.461	1.00 20.80	A
	ATOM	278	CB			107		37.779	5.694	-2.337	1.00 22.93	A
	MOTA	279	CG			107		36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD			107		35.431	5.975	-3.148	1.00 32.40	A
15	MOTA	281		GLU				35.262	6.939	-3.923	1.00 33.74	A
	MOTA	282	OE2					34.608	5.654	-2.263	1.00 36.00	A
•	MOTA	283	C			107		40.053	5.678	-1.410	1.00 18.93	A
	ATOM	284	0			107		39.891	5.427	-0.220	1.00 19.21	A
	MOTA	285	N			108		40.988	6.507	-1.852	1.00 16.70	A
20	MOTA	286	CA			108		41.883	7.209	-0.942	1.00 15.86	A
	MOTA	287	CB			108		43.325	6.728	-1.104	1.00 15.30	A
	MOTA	288	CG			108		43.593	5.328	-0.612	1.00 16.33 1.00 16.36	A A
	MOTA	289		TYR				43.765	5.066	0.746		A
	MOTA	290		TYR				44.046	3.769	1.201	1.00 18.48 1.00 13.25	A
25	MOTA	291		TYR				43.701	4.268	-1.511	1.00 13.23	A
	ATOM	292		TYR				43.980	2.981	-1.075 0.276	1.00 17.28	A
	ATOM	293	CZ			108	1	44.152	2.736	0.278	1.00 19.17	A
	ATOM	294	ОН			108		44.440 41.850	1.461 8.687	-1.292	1.00 16.80	Α
20	ATOM	295	C			108		41.550	9.058	-2.431	1.00 15.22	A
30	ATOM	296	. O			108 109		42.132	9.528	-0.306	1.00 13.22	A
	ATOM	297	N			109		42.132	10.957	-0.539	1.00 14.30	A
	ATOM	298 299	CA CB			109		41.671	11.726	0.661	1.00 14.78	A
	ATOM ATOM	300	C			109		43.713	11.136	-0.667	1.00 16.79	A
35	ATOM ,	301	0			109		44.450	10.983	0.317	1.00 16.52	A
33	ATOM	302	И			110		44.182	11.410	-1.881	1.00 14.80	A
	ATOM	303	CA			110		45.609	11.574	-2.093	1.00 15.80	A
	ATOM	304	CB			110		46.065	10.863	-3.396	1.00 16.85	A
	ATOM	305		ILE				47.550	11.098	-3.632	1.00 16.80	A
40	ATOM	306		ILE				45.774	9.358	-3.284	1.00 17.76	Α
,,	ATOM	307		ILE				46.308	8.513	-4.437	1.00 16.07	A
	ATOM	308	C			110		46.004	13.045	-2.129	1.00 17.78	Α
	ATOM	309	Ō			110		45.534	13.813	-2.976	1.00 16.24	A
	ATOM	310	N	LYS	Α	111		46.846	13.435	-1.177	1.00 16.15	. A
45	ATOM	311	CA	LYS	Α	111		47.326	14.808	-1.100	1.00 17.20	Α
	ATOM	312	CB			111		47.700	15.176	0.344	1.00 17.41	A
	MOTA	313	CG	LYS	A	111		48.350	16.547	0.464	1.00 20.71	. A
	ATOM	314	CD	LYS	Α	111		48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE	LYS	Α	111		47.288	17.381	2.598	1.00 29.46	A
50°	ATOM	316	NZ	LYS	Α	111		47.516	17.866	4.000	1.00 30.50	Α
	ATOM	317	С	LYS	A	111	•	48.551	14.890	-1.994	1.00 16.41	Α
	MOTA	318	0			111		49.509	14.137	-1.813	1.00 18.20	A
	ATOM	319	N	ILE	A	112		48.509	15.798	-2.963	1.00 15.87	A
	MOTA	320	CA	ILE	A	112		49.606	15.967	-3.907	1.00 17.28	A:
55	ATOM	321	CB			112		49.079	15.911	-5.358	1.00 16.43	Α.
	MOTA	322		ILE				50.235	15.998	-6.341	1.00 15.12	A
	MOTA	323		ILE				48.293	14.609	-5.565	1.00 16.82	A
	MOTA	324		ILE				47.580	14.511	-6.904	1.00 18.47	A
	MOTA	325	С	ILE	Α	112		50.307	17.301	-3.663	1.00 19.03	A

	ATOM	326	0	ILE	Α	112		49.669	18.350	-3.635	1.00 19.15	A
	ATOM	327	N	LEU	Α	113		51.622	17.245	-3.472	1.00 20.22	A
	ATOM	328	CA	LEU	Α	113		52.416	18.442	-3.214	1.00 22.36	A
	ATOM	329	СВ	LEU	Α	113		52.995	18.397	-1.794	1.00 22.13	A
5	ATOM	330	CG	LEU	Α	113		52.042	18.063	-0.646	1.00 22.46	A
. (ATOM	331	CD1	LEU	Α	113		51.866	16.557	-0.553	1.00 23.81	A
	ATOM	332		LEU				52.603	18.595	0.660	1.00 23.68	A
	ATOM	333	С	LEU				53.560	18.547	-4.215	1.00 23.37	A
	ATOM	334	0	LEU				54.300	17.586	-4.424	1.00 23.11	A
10	ATOM	335	N	GLU				53.706	19.714	-4.834	1.00 23.88	A
	ATOM	336	CA	GLU				54.771	19.920	-5.806	1.00 26.00	A
	ATOM	337	CB	GLU				54.435	21.111	-6.706	1.00 27.74	A
	ATOM	338	CG	GLU				55.533	21.452	-7.696	1.00 35.07	A
	ATOM	339	CD	GLU				55.220	22.696	-8.497	1.00 39.24	A
15	ATOM	340		GLU				54.808	23.703	-7.885	1.00 41.45	A
13	ATOM	341		GLU				55.395	22.670	-9.736	1.00 44.05	A
	ATOM	342	C	GLU				56.087	20.163	-5.067	1.00 24.37	A
	MOTA	343	0	GLU				56.186	21.071	-4.238	1.00 24.43	A
	ATOM	344	N	LYS				57.096	19.350	-5.360	1.00 24.10	A
20	ATOM	345	CA	LYS				58.376	19.493	-4.678	1.00 24.10	A
20	ATOM	346	CB	LYS				59.339	18.373	-5.103	1.00 23.72	A
		347	CG	LYS				59.139	17.080	-4.308	1.00 23.72	A
	MOTA MOTA	348	CD	LYS				60.064	15.944	-4.743	1.00 21.92	A
	ATOM	349	CE	LYS				59.691	15.400	-6.117	1.00 22.42	A
25	ATOM	350	NZ	LYS				60.447	14.150	-6.448	1.00 22.42	A
23	ATOM	351	C	LYS				59.031	20.858	-4.868	1.00 15.71	A
	ATOM	352	0	LYS				59.492	21.469	-3.903	1.00 26.17	A
	ATOM	353	N	ARG				59.058	21.348	-6.102	1.00 28.73	A
	ATOM	354	CA	ARG				59.678	22.638	-6.380	1.00 29.66	A
30	ATOM	355	CB.	ARG				59.533	22.980	-7.868	1.00 31.29	. A
50	ATOM	356	CG	ARG				60.047	24.361	-8.267	1.00 33.19	A
	ATOM	357	CD	ARG				61.368	24.710	-7.590	1.00 35.13	A
	ATOM	358	NE	ARG				62.329	23.612	-7.618	1.00 36.42	A
	ATOM	359	CZ	ARG				63.510	23.648	-7.019	1.00 36.18	A
35	ATOM	360		ARG				63.871	24.729	-6.332	1.00 36.12	A
23	ATOM	361		ARG				64.324	22.602	-7.067	1.00 35.77	A
	ATOM	362	C	ARG				59.097	23.761	-5.519	1.00 29.70	A
	ATOM	363	0	ARG				59.843	24.515	-4.889	1.00 29.16	A
	ATOM	364	N	HIS				57.773	23.862	-5.472	1.00 27.22	A
40	ATOM	365	CA	HIS				57.126	24.903	-4.681	1.00 27.22	A
40	ATOM	366	CB	HIS				55.606	24.835	-4.848	1.00 28.41	A
	ATOM	367	CG	HIS				54.881	26.005	-4.258	1.00 20.11	A
	ATOM	368		HIS			•	55.309	27.249	-3.935	1.00 33.19	A
	ATOM	369		HIS				53.536	25.974	-3.961	1.00 34.30	A
45	ATOM	370		HIS				53.165		-3.480	1.00 34.58	A
43	ATOM	371		HIS				54.222	27.940	-3.455	1.00 35.18	· A
	ATOM	372	C	HIS				57.477	24.780	-3.202	1.00 26.22	A
	MOTA	373	0	HIS				57.737	25.776	-2.534	1.00 25.67	A
	ATOM	374	N	ILE				57.469	23.770	-2.689	1.00 24.94	A
50	ATOM	375	CA	ILE				57.792	23.334	-1.285	1.00 23.94	A
50	ATOM	376	CB	ILE				57.711	21.812	-0.952	1.00 23.50	Α
	ATOM	377		ILE				58.374	21.533	0.389	1.00 23.76	A
	ATOM	378		ILE				56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379		ILE				56.066	19.858	-0.834	1.00 28.06	A
55	ATOM	380	CDI	ILE				59.195	23.821	-0.958	1.00 23.78	A
,,	ATOM	381	Ö	ILE				59.402	24.495	0.048	1.00 23.49	A
	ATOM	382	N	ILE				60.153	23.489	-1.815	1.00 23.46	A
	MOTA	383	CA	ILE				61.534	23.913	-1.619	1.00 25.13	A
	ATOM	384	CB			119		62.467	23.250	-2.664	1.00 24.25	A
	0	201	25					Ju. 10/	20.200	2.001	· · -	

	MOTA	385	CG2	ILE	A	119		63.	858	23.89	90	-2.617	1.00	22.47	A
	ATOM	386	CG1	ILE	Α	119		62.	540	21.73		-2.395		25.05	A
	ATOM	387	CD1	ILE	A	119		63.	327	20.94	5	-3.439		24.62	A
	ATOM	388	C	ILE	A	119		61.	667	25.43		-1.705		25.96	A
′ 5	ATOM	389	0	ILE	A	119		62.	330	26.05		-0.872		24.78	A
	ATOM	390	N	LYS	A	120		61.	028	26.03		-2.704		27.67	A
	ATOM	391	CA	LYS	Α	120		61.	100	27.48	39.	-2.879		30.29	A
	ATOM	392	CB	LYS	Α	120		60.	242	27.94	łO	-4.060		32.34	A
	ATOM	393	CG	LYS	Α	120		60.	674	27.40	7	-5.409		39.30	A
10	MOTA	394	CD	LYS	Α	120		59	.765	27.95		-6.512		45.19	A
	MOTA	395	CE	LYS	A	120		58	.294	27.63	36	-6.218	1.00	46.48	A
	MOTA	396	NZ	LYS	A	120		57	.363	28.15	55	-7.252	1.00	46.49	A
	MOTA	397	C.	LYS	Α	120		60.	647	28.24	17	-1.638	1.00	30.89	A
	MOTA	398	0	LYS	Α	120		61	.303	29.19	98	-1.217	1.00	32.48	A
15	MOTA	399	N	GLU	Α	121		59	.527	27.82	25	-1.055	1.00	29.82	A
	ATOM	400	CA	GLU.	Α	121		58	.986	28.48	88	0.128	1.00	30.33	A
	ATOM	401	CB	GLU	Α	121		57	. 455	28.41	16	0.117	1.00	33.04	A
	ATOM	402	CG	GLU	Α	121		56	.794	29.02	21	-1.120	1.00	36.45	A
	ATOM	403	CD	GLU	A	121		57	.221	30.45	56	-1.373	1.00	39.88	A
20	ATOM	404	OE1	GLU	A	121		57	.200	31.26	54	-0.420	1.00	40.53	A
	ATOM	405	OE2	GLU	Α	121		57	.573	30.77	78	-2.529	1.00	43.24	A
	ATOM	406	С	GLU	Α	121		59	.511	27.93	30	1.451	1.00	30.37	A
	MOTA	407	0	GLU	Α	121		58	.946	28.20	04	2.513	1.00	31.24	A
	ATOM	408	N	ASN	Α	122		60	.588	27.15	51	1.390	1.00	29.03	A
25	MOTA	409	CA	ASN	Α	122		61	.183	26.57	73	2.594	1.00	28.46	A
	MOTA	410	CB	ASN	A	122		61	.836	27.67	73	3.436	1.00	31.28	A
	ATOM	411	CG	ASN	Α	122		62	.945	28.39	95	2.698	1.00	34.12	A
	ATOM	412	OD1	ASN	Α	122		62	.697	29.14	43	1.754	1.00	35.57	A
	MOTA	413	ND2	ASN	А	122		64	.181	28.16	69	3.127	1.00	35.73	A
30	ATOM	414	C	ASN	Α	122		60	.157	25.83	35	3.456	1.00	26.89	A
	ATOM	415	0	ASN	Α	122		60	.085	26.05	55	4.663	1.00	27.23	A
	MOTA	416	N	LYS	A	123		59	.375	24.95	55	2.842	1.00	23.99	A
	MOTA	417	CA	LYS	Α	123		58	.358	24.2	10	3.574	1.00	22.43	A
	MOTA	418	CB	LYS	Α	123		57	.031	24.24	48	2.810	1.00	21.97	A
35	ATOM	419	CG	LYS	Α	123		56	.475	25.64	45	2.599	1.00	25.68	A
	ATOM	420	CD	LYS	Α	123		56	.253	26.35	54	3.927	1.00	27.54	· А
	ATOM	421	CE	LYS	Α	123		55	.822	27.79	96	3.716	1.00	31.30	Α
	MOTA	422	NZ	LYS	Α	123		55	.756	28.54	40	5.004	1.00	33.21	, A.
	ATOM	423	С	LYS	Α	123		58	.748	22.75	59	3.821	1.00	22.20	Α
40	ATOM	424	0	LYS	Α	123		57	.924	21.9	60	4.264	1.00	22.50	A
	MOTA	425	N	VAL	A	124		59	.997	22.4	12	3.535	1.00	20.59	A
	ATOM	426	CA	VAL	Α	124		60	.439	21.0	39	3.730	1.00	20.25	A
*	ATOM	427	CB	VAL	Α	124		61	.922	20.8	50	3.328	1.00	19.43	· A
	ATOM	428	CG1	VAL	Α	124		62	.346	19.4	07	3.573	1.00	18.69	A
45	ATOM	429	CG2	VAL	Α	124		62	.104	21.1	95	1.853	1.00	18.21	A
	ATOM	430	C			124			.236	20.5	61	5.163	1.00	19.53	A
	ATOM	431	0	VAL	Α	124		59	.841	19.4	18	5.385	1.00	20.02	A
	ATOM	432	N			125		60	.513	21.4	22	6.159	1.00	20.01	A
	ATOM	433	CD	PRO	Α	125		61	.178	22.7	38	6.118	1.00	18.69	.A.
50	ATOM	434	CA	PRO	Α	125		60	.318	20.9	79	7.544	1.00	19.88	Α
	ATOM	435	CB			125		60	.793	22.1	80	8.363	1.00	19.95	A
	ATOM	436	CG			125		61	.839	22.8	05	7.479	1.00	18.85	A
	MOTA	437	C			125		58	.848	20.6	42	7.824		19.76	Α
	ATOM	438	0			125		58	.544	19.7	00	8.550	1.00	16.99	A
55	MOTA	439	N			126		57	.947	21.4	18	7.235	1.00	18.98	A
	ATOM	440	CA			126			.516	21.2	20	7.435		21.97	A
	ATOM	441	CB			126	-		.752	22.4	48	6.933		25.17	A
	MOTA	442	CG			126			.040	23.6	90	7.748		30.98	A
	MOTA	443		TYR					.438	23.8	86	8.991	1.0	33.95	A

	ATOM	444	CE1	TYR	A	126	9	55.721	25	.015	9.763	1.00	36.60	A
	MOTA	445	CD2	TYR	A	126	5	6.938	24	1.657	7.292	.1.00	35.43	A
	ATOM	446	CE2	TYR	Α	126		57.231	25	5.792	8.058	1.00	37.20	A
	MOTA	447	CZ	TYR	А	126		66.618	25	5.962	9.291	1.00	37.40	A
5	ATOM	448	ОН	TYR	Α	126		56.903	27	7.073	10.052	1.00	40.85	A
-	ATOM	449	C	TYR			9	55.990	19	9.956	6.762	1.00	21.35	A
	ATOM	450	ō	TYR			9	55.265	19	9.175	7.383	1.00	20.49	A
	ATOM	451	N	VAL				56.354		9.746	5.501	1.00	18.16	A
	ATOM	452	CA	VAL				55.892		3.562	4.790	1.00	17.58	A
10	ATOM	453	CB	VAL				56.308		3.596	3.308	1.00	17.45	A
10	ATOM	454		VAL				55.786		7.350	2.600		17.97	A
	ATOM	455	CG2	VAL				55.751		9.850	2.641		14.90	A
	ATOM	456	C	VAL				56.459		7.306	5.448		18.39	A
		457	0	VAL				55.769		5.298	5.583		18.14	A
15	ATOM			THR				57.716		7.381	5.869		17.50	Α
15	MOTA	458	N	THR				58.375		5.260	6.530		18.54	A
	MOTA	. 459	CA					59.861			6.805		18.01	A
	ATOM	460	CB	THR						5.804	5.559		21.14	A
	ATOM	461		THR				60.537			7.545		17.95	A
	ATOM	462	CG2	THR				60.536		5.446			19.49	A
20	ATOM	463	C	THR				57.676		5.941	7.856			A
	ATOM	464	0	THR				57.438		1.776	8.179		18.76	
	MOTA	465	N	ARG				57.345		5.981	8.619		19.60	A
	MOTA	466	CA	ARG				56.673		5.804	9.904		20.12	A
	MOTA	467	CB	ARG				56.534		8.144	10.621		21.33	A
25	ATOM	468	CG	ARG				55.948		B.029	12.023		28.02	. A
	ATOM	469	$^{\rm CD}$	ARG				55.721		9.404	12.597		31.25	A
	MOTA	470	NE	ARG	Α	129		56.940		0.205	12.560		37.78	A
	MOTA	471	CZ	ARG	Α	129	•	56.962		1.524	12.391		40.10	A
	MOTA	472	NH1	ARG	A	129		55.828	2:	2.197	12.239		40.03	A
30	MOTA	473	NH2	ARG	Α	129		58.119	2	2.170	12.374		44.58	A
	MOTA	474	C	ARG	A	129		55.288	1	6.186	9.729		20.08	A
	MOTA	475	0	ARG	А	129		54.891	1.	5.305	10.496		20.40	· A
	MOTA	476	N	GLU	А	130		54.553	1	6.654	8.724	1.00	18.79	A
	ATOM	477	CA	\mathtt{GLU}	A	130		53.222	1	6.125	8.454	1.00	20.10	Α
35	MOTA	478	CB	GLU	Α	130		52.638	1	6.749	7.183	1.00	19.92	A
	MOTA	479	CG	GLU	Α	130		51.350	1	6.087	6.708	1.00	27.85	A
	MOTA	480	CD	GLU	A	130		50.581	. 1	6.933	5.707	1.00	29.72	A
	MOTA	481	OE1	GLU	Α	130		51.216	1	7.528	4.814	1.00	33.46	A
	ATOM	482	OE2	GLU	Α	130		49.339	1	6.996	5.807	1.00	30.74	A
40	MOTA	483	C	GLU	Α	130		53.301	. 1	4.615	8.295	1.00	19.81	A
	ATOM	484	0	GLU	Α	130		52.553	1	3.875	8.935	1.00	18.37	A
	MOTA	485	N	ARG	Α	131		54.219	1	4.162	7.447	1.00	20.41	A
	ATOM	486	CA	ARG	Α	131	•	54.397	1	2.735	7.202	1.00	22.45	A
	ATOM	487	CB	ARG	A	131		55.442	1	2.511	6.098	1.00	25.16	A
45	ATOM	488	CG	ARG	Α	131		55.742	1	1.043	5.840	1.00	28.75	Α
	ATOM	489	CD			131		56.736		0.837	4.708	1.00	33.75	A
	ATOM	490	NE			131		57.020		9.415	4.520	1.00	40.07	A
	ATOM	491	CZ			131		57.756		8.915	3.532	1.00	43.07	A
	ATOM	492		ARG				58.293		9.721	2.625		44.91	A
50	ATOM	493		ARG				57.955		7.606	3.449	1.00	44.45	A
50	ATOM	494	C			131		54.820		1.982	8.466		23.24	Ā
	ATOM	495	o			131		54.241		0.948	8.804		23.86	A
	ATOM	496	N			132		55.831		2.497	9.160		21.99	A
	ATOM	490	CA			132		56.318		1.850	10.370		22.04	A
55		497	CB			132		57.570		2.564	10.888		23.72	A
رر	MOTA	498	CG			132		58.750		2.442	9.932		27.77	A
	ATOM			ASP				58.681		1.620			27.34	A
	ATOM	500		ASP				59.753		3.163	10.128		28.70	A
	ATOM	501				132		55.258		1.772	11.474		21.69	A
	MOTA	502	С	HOP	А	132		JJ. ZJ0	, 1	/ / 2	TT. 4	1.00		

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	MOTA	503	0	ASP,	Α	132	55.077	10.723	12.092	1.00 22.75	Α
	MOTA	504	N	VAL	Α	133	54.551	12.868	11.725	1.00 19.54	A
	MOTA	505	CA	VAL	A	133	53.525	12.843	12.759	1.00 18.52	A
	ATOM .	506	CB	VAL	A	133	52.908	14.244	12.990	1.00 19.26	A
5	ATOM	507		VAL			51.708	14.135	13.918	1.00 18.79	A
	MOTA	508	CG2	VAL	Α	133	53.953	15.180	13.604	1.00 18.80	A
	ATOM	509	C	VAL	Α	133	52.419	11.854	12.398	1.00 19.46	A
	ATOM	510	0	VAL	Α	133	52.073	10.991	13.200	1.00 19.94	A
	ATOM	511	N	MET	A	134	51.878	11.957	11.187	1.00 19.15	A
10	ATOM	512	CA	MET			50.807	11.052	10.792	1.00 21.25	A
	MOTA	513	CB	MET			50.309	11.381	9.383	1.00 17.34	A
	ATOM	514	CG	MET			49.615	12.730	9.302	1.00 20.00	A
	ATOM	515	SD	MET			48.643	12.952	7.798	1.00 24.21	A
	ATOM	516	CE	MET			47.033	12.434	8.400	1.00 23.20	A
15	MOTA	517	C	MET			51.203	9.582	10.881	1.00 22.43	A
	ATOM	518	0	MET			50.384	8.741	11.249	1.00 23.82	A
	MOTA	519	N .	SER			52.454	9.273	10.556	1.00 23.09	A
	ATOM	520	CA	SER			52.939	7.895	10.615	1.00 26.13	A
	MOTA	521	CB	SER			54.356	7.798	10.039	1.00 26.17	A
20	MOTA	522	OG	SER			54.383	8.177	8.673	1.00 31.91 1.00 26.58	A A
	ATOM	523	C	SER			52.957	7.358	12.045	1.00 26.38	A
	ATOM	524	0	SER			52.926	6.148 8.261	12.261 13.018	1.00 25.42	A
	MOTA	525 526	N	ARG ARG			53.014 53.056	7.870	14.425	1.00 23.63	A
25	ATOM	526 527	CA CB	ARG			53.823	8.914	15.238	1.00 27.47	A
23	MOTA	52 <i>1</i> 528	CG	ARG			55.283	9.082	14.857	1.00 32.00	A
	ATOM ATOM	526 529	CD	ARG			55.904	10.218	15.664	1.00 32.00	A
	ATOM	530	NE	ARG			55.602	10.213	17.084	1.00 36.11	A
	ATOM	531	CZ	ARG			55.867	10.990	18.007	1.00 39.74	A
30	ATOM	532				136	56.449	12.132	17.661	1.00 40.55	A
50	ATOM	533		ARG			55.540	10.769	19.276	1.00 36.72	A
•	MOTA	534	C	ARG			51.667	7.709	15.036	1.00 26.38	A
	ATOM	535	ō	ARG			51.516	7.121	16.106	1.00 27.06	A
	ATOM	536	N	LEU			50.655	8.235	14.360	1.00 24.77	A
35	ATOM	537	CA	LEU			49.294	8.162	14.870	1.00 24.70	A
	ATOM	538	CB	LEU	А	137	48.483	9.363	14.371	1.00 24.52	A
	MOTA	539	CG.	LEU	Α	137	49.050	10.760	14.662	1.00 26.67	A
	ATOM	540	CD1	LEU	Α	137	48.075	11.813	14.141	1.00 27.25	A
	ATOM	541	CD2	LEU	Α	137	49.279	10.945	16.155	1.00 27.09	A
40	ATOM	542	С	LEU	A	137	48.592	6.868	14.473	1.00 25.20	A
	ATOM	543	0	LEU	A	137	48.619	6.469	13.309	1.00 25.99	A
	ATOM	544	N	ASP	Α	138	47.971	6.218	15.451	1.00 21.89	A
	ATOM	545	CA	ASP	А	138	47.239	4.977	15.219	1.00 21.35	A
	ATOM	546	CB	ASP	Α	138	48.124	3.761	15.523	1.00 22.14	A
45	.ATOM	547	CG	ASP	Α	138	47.432	2.448	15.201	1.00 24.90	A
	MOTA	548		ASP			46.631	2.423	14.241	1.00 24.78	Α
	ATOM	549	OD2	ASP			47.691	1.443	15.897	1.00 25.39	A
	MOTA	550	С	ASP			46.031	4.991	16.138	1.00 20.47	A
	ATOM	551	0	ASP			45.967	4.248	17.118	1.00 19.06	A
50	MOTA	552	N	HIS			45.075	5.852	15.810	1.00 18.27	A
	MOTA	553	CA	HIS			43.869	6.016	16.606	1.00 18.21	A
	ATOM	554	CB	HIS			44.096	7.157	17.612	1.00 15.84	A
	ATOM	555	CG	HIS			42.985	7.332	18.600	1.00 15.24	A N
	ATOM	556		HIS			42.884	6.964	19.900	1.00 13.97	A
55	ATOM	557		HIS			41.791	7.943	18.280	1.00 14.74	, A A
	MOTA	558 550		HIS			41.002	7.944	19.341	1.00 14.19	A
	MOTA	559 560		HIS			41.641	7.356 6.330	20.336	1.00 14.15	A
	MOTA	560 561	C			139	42.715 42.879	7.080	15.654 14.693	1.00 18.50	A
	MOTA	561	0	ura	А	139	12.079	7.000	12.023	1.00 20.00	*3

	ATOM	562	N	PRO	Α	140	4	1.527	7	5.767	15.913	1.00	18.32	A
	ATOM	563	CD	PRO	Α	140	4	1.143	3	4.984	17.100	1.00	16.71	A
	MOTA	564	CA	PRO	Α	140	4	0.367	7	6.001	15.048	1.00	17.43	A
	ATOM	565	CB	PRO	Α	140	3	9.273	3	5.157	15.704	1.00	16.64	A
5	MOTA	566	CG	PRO	А	140	3	9.643	3	5.204	17.152		18.43	A
	MOTA	567	C	PRO	А	140	3	9.914	1	7.441	14.80		18.77	A
	MOTA	568	0	PRO	A	140	3	9.207	7	7.695	13.83		19.88	A
	ATOM	569	И	PHE	Α	141	4	0.30	1	8.381	15.664		17.14	A
	ATOM	570	CA	PHE	Α	141	3	9.874	4	9.767	15.47		16.42	A
10	ATOM	571	CB	PHE	Α	141	3	9.568	В	10.422	16.83		14.60	A
	ATOM	572	CG	PHE	A	141	3	8.386	5	9.817	17.55		15.26	A
	MOTA	573	CD1	PHE	A	141	3	7.335	5	9.234	16.842		14.78	A
	MOTA	574	CD2	PHE	A	141	3	8.29	7	9.880	18.942		13.70	A
	ATOM	575	CE1	PHE	Α	141	3	6.215	5	8.727	17.50		16.94	A
15	MOTA	576	CE2	PHE	A	141	3	7.178	В	9.375	19.61	_	15.75	A
	MOTA	577	CZ	PHĖ	A	141	` 3	6.13	5	8.799	18.89		16.89	Α
	MOTA	578	C	PHE	Α	141	4	0.85	7	10.641	14.69		16.15	A
	MOTA	579	0	PHE	A	141	4	0.799	9	11.871	14.76		17.35	A
	MOTA	580	N	PHE	A	142	. 4	1.748	В	10.011	13.94		15.88	A
20	MOTA	581	CA	PHE	Α	142	4	2.72		10.756	13.15		17.89	A
	MOTA	582	CB	PHE	Α	142	4	4.11!	5	10.645	- 13.79		17.57	A
	MOTA	583	CG	PHE	Α	142	4	4.24	0	11.371	15.10		18.74	A
	ATOM	584	CD1	PHE	Α	142	4	4.55	9	12.726	15.13		17.77	A
	MOTA	585	CD2	PHE	Α	142	4	3.99	7	10.711	16.30		18.74	A
25	MOTA	586	CE1	PHE	А	142	4	4.632	2	13.417	16.34		15.77	Ą
	MOTA	587	CE2	PHE	Α	142	4	4.06	5	11.393	17.52		17.56	A
	MOTA	588	CZ	PHE	A	142	4	4.383	3	12.747	17.54		17.14	A
•	MOTA	589	С	PHE	Α	142	4	2.79	3	10.231	11.72		19.12	A
•	MOTA	590	0	PHE	A	142	4	2.65	9	9.030	11.50		20.01	A
30	MOTA	591	N	VAL				2.97		11.135	10.76		18.72	A
	MOTA	592	CA	VAL				3.10		10.735	9.37		18.52	A
	MOTA	593	CB	VAL				3.29		11.961	8.44		20.66	A
	MOTA	594		VAL				3.84		11.521	7.08		21.29	A
	ATOM	595		VAL				1.95		12.673	8.25		22.97	A
35	MOTA	' 596	C			143		4.34		9.865	9.33		18.68	A
	MOTA	597	0	VAL				5.35		10.199	9.94		18.42	A
	ATOM	598	N			144		4.25		8.745	8.62		18.30	A
	MOTA	599	CA	LYS				5.38		7.824	8.53	-	18.78	. A
	ATOM	600	CB			144		4.88		6.373	8.60		22.27	A
40	ATOM	601	CG			144		6.01		5.340	8.55		29.72	A
	ATOM	602	CD			144		5.49		3.912	8.67		34.16	A
	MOTA	603	CE			144		6.63		2.896	8.57		37.67	A N
	ATOM	604	NZ			144		6.13		1.484	8.62		39.02	A A
	ATOM	605	C			144		6.19		8.002	7.26		18.53	
45	MOTA	606	0	LYS				5.64		8.314	6.20		18.18	A n
	MOTA	607	N			145		7.50		7.816	7.38		16.79 17.45	A A
	ATOM	608	CA			145		8.41		7.900	6.25			A
•	ATOM	609	CB			145		9.68		8.653	6.64 5.54		18.82	A
	ATOM	610	CG			145		0.73		8.902			18.83	A
50	ATOM	611 '		LEU				1.83		9.799	6.09		19.79	A
	MOTA	612		LEU				1.31		7.581	5.06		19.19	A
	MOTA	613	C			145		8.73		6.450	5.90		17.36	· A
	MOTA	614	0			145		9.45		5.772	6.65		17.38	A
	ATOM	615	N			146		8.21		5.972 4.593	4.78 4.35		17.20	A
55	MOTA	616	CA			146		8.44 7.28		4.593	3.48		17.74	A
	MOTA	617 618	CB			146		5.98		3.926	4.21		17.50	
	MOTA	618	CG			146		15.90		4.995	4.21		16.50	A
	MOTA	619 620		TYR				13.88		4.827	5.03		17.10	A
	MOTA	620	CEI	TYR	A	140	4		_	7.04/	٥.٠٥	J 1.00	, 1,.10	••

	ATOM	621	CD2	TYR	Α	146	45.620	2.686	4.735	1.00	18.28	A
	MOTA	622	CE2	TYR	A	146	44.411	2.506	5.399	1.00	19.84	A
	MOTA	623	CZ	TYR	A	146	43.547	3.576	5.544	1.00	17.53	Α
	ATOM	624	OH	TYR			42.342	3.376	6.169		20.67	. A
5	MOTA	625	C	TYR	A	146	49.735	4.376	3.582		18.72	A
	MOTA	626	0	TYR			50.382	3.338	3.715		19.51	A
	ATOM	627	N	PHE	A	147	50.110	5.350	2.765		18.09	A
	MOTA	628	CA	PHE			51.307	5.203	1.952		17.20	A
	MOTA	629	CB	PHE			51.007	4.258	0.783		16.77	A
10	MOTA	630	CG	PHE			49.835	4.699	-0.070		17.75	A
	MOTA	631		PHE			49.967	5.752	-0.975		16.58	A
	MOTA	632		PHE			48.595	4.075	0.053		18.07	A
	MOTA	633		PHE			48.886	6.178	-1.742		19.62	A
	MOTA	634		PHE			47.503	4.492	-0.710		18.56	A
15	MOTA	635	CZ			147	47.647	5.546	-1.610		19.27	A
	MOTA	636	С			147	51.768	6.533	1.395		17.13	A
	ATOM	637	0			147	51.045	7.528	1.452		14.43	· A
-	ATOM .	638	N			148	52.981	6.534	0.854		17.12	A
•	ATOM	639	CA			148	53.541	7.718	0.232		17.96	A
20	ATOM	640	CB			148	54.449	8.531	1.197		21.51	A
	MOTA	641		THR			55.605	7.760	1.537		18.83	A
	ATOM	642	CG2	THR			53.700	8.897	2.472 -0.946		19.60 20.31	A A
	MOTA	643	C			148	- 54.386	7.262	-0.946		18.94	A
25	ATOM	644	O N			148	54.860 54.543	6.124	-1.916		19.16	A
25	ATOM ATOM	645 646	N CA			149 149	55.368	8.149 7.877	-3.073		18.01	A
	ATOM	647	CB			149	54.748	6.801	-3.989		17.23	A
	ATOM	648	CG			149	53.389	7.144	-4.544		16.88	· A
	ATOM	649		PHE			53.262	7.888	-5.712		18.58	A
30	ATOM	650		PHE			52.235	6.668	-3.927		17.31	A
50	ATOM	651		PHE			52.007	8.149	-6.267		19.26	A
	ATOM	652		PHE			50.972	6.923	-4.470		19.17	A
	ATOM	653	CZ			149	50.858	7.663	-5.642		19.60	A
	ATOM	654	C			149	55.542	9.205	-3.774		20.85	A
35	ATOM	655	ō			149	54.934	10.200	-3.376		19.76	A
•	ATOM	656	N			150	56.398	9.241	-4.782		19.79	A
	ATOM	657	CA	GLN			56.636	10.481	-5.497		24.03	A
-	ATOM	658	CB			150	57.659	11.347	-4.739	1.00	24.45	A
	ATOM	659	CG			150	58.986	10.645	-4.414	1.00	26.28	Α
40	MOTA	660	CD	GLN	Α	150	59.988	11.558	-3.692	1.00	29.02	A
	ATOM	661	OE1	GLN	А	150	60.693	12.353	-4.321	1.00	27.05	A
	ATOM	662	NE2	GLN	А	150	60.042	11.449	-2.365	1.00	26.47	A
	ATOM	663	C	GLN	Α	150	57.160	10.203	-6.885	1:00	23.88	A
	MOTA	664	0	GLN	Α	150	57.673	9.118	-7.158	1.00	24.79	A
45	MOTA	665	N	ASP	Α	151	56.987	11.171	-7.774	1.00	25.88	A
	MOTA	666	CA	ASP	Α	151	57.527	11.047	-9.117	1.00	26.49	A
	ATOM	667	CB	ASP	A	151	56.437	11.126	-10.199	1.00	24.54	A
	MOTA	668	CG	ASP	Α	151	55.544	12.336	-10.064	1.00	24.95	A
	MOTA	669	OD1	ASP	A	151	56.005	13.379	-9.561	1.00	22.44	A
50	MOTA	670	OD2	ASP	A	151	54.369	12.242	-10.490		25.72	A
	MOTA	671	C			151	58.515	12.203	-9.220		28.63	A
	ATOM	672	0			151	58.890	12.780	-,8.194		27.83	A
	ATOM	673	N			152	58.934		-10.426		29.21	A
	ATOM	674	CA			152	59.907		-10.562		31.88	A
55	ATOM	675	CB			152	60.325		-12.026		33.94	A
	ATOM	676	CG			152	61.033		-12.557		38.88	A
	ATOM	677		ASP			61.817		-11.791		39.67	A
	ATOM	678		ASP			60.817		-13.738		41.57	A
	MOTA	679	C	ASP	Α	152	59.487	14.994	-10.013	1.00	30.90	A

	ATOM	680	0	ASP	Α	152	60.316	15.735	-9.482	1.00	31.69	A
	ATOM	681	N	GLU			58.207	15.322	-10.107	1.00	29.44	A
	ATOM	682	CA	GLU			57.767	16.632	-9.646	1.00	28.69	Α
	ATOM	683	СВ	GLÜ			56.984		-10.766	1.00	32.90	Α
5	ATOM	684	CG	GLU			57.451		-12.183		40.57	· A
_	ATOM	685	CD	GLU			56.920		-12.675		45.78	A
	ATOM	686		GLU			55.682		-12.760		48.91	A
	ATOM	687		GLU			57.736		-12.979		48.95	A
			C				56.929	16.683	-8.372		26.43	A
10	ATOM	688		GLU			56.947	17.688	-7.660		25.08	A
10	ATOM	689	0	GLU					-8.069		22.39	A
	ATOM	690	N	LYS			56.205	15.610				A
	ATOM	691	CA	LYS			55.318	15.631	~6.912		21.43	
	MOTA	692	CB	LYS			53.861	15.628	-7.398		20.33	A
	ATOM	693	CG	LYS			53.505	16.716	-8.403		21.92	A
15	MOTA	694	CD	LYS			52.211	16.375	-9.146		19.70	A
	ATOM	695	CE	LYS	A	154	51.775		-10.077		20.04	A
	ATOM	696	NZ	LYS	Α	154	50.631	17.094	-10.951	1.00	19.97	A
	MOTA	697	C	LYS	A	154	55.458	14.522	-5.881	1.00	20.43	A
	MOTA	698	0	LYS	Α	154	55.949	13.426	-6.173	1.00	21.13	A
20	MOTA	699	N	LEU	Α	155	54.985	14.832	-4.676	1.00	19.69	A
	MOTA	700	CA	LEU	Α	155	54.950	13.900	-3.553	1.00	19.10	A
	MOTA	701	CB	LEU	Α	155	55.362	14.588	-2.252	1.00	19.65	A
	ATOM	702	CG	LEU	Α	155	56.740	15.234	-2.129	1.00	21.20	A
	ATOM	703	CD1	LEU	Α	155	56.848	15.918	-0.770	1.00	23.42	A
25	ATOM	704		LEU			57.816	14.174	-2.277	1.00	23.08	A
	ATOM	705	С	LEU			53.478	13.507	-3.427	1.00	18.87	A
	ATOM	706	ō			155	52.600	14.348	-3.620		18.61	A
	ATOM	707	N	TYR			53.209	12.249	-3.091		15.02	A
	ATOM	708	CA	TYR			51.834	11.783	-2.934		16.29	A
30	ATOM	709	CB			156	51.470	10.769	-4.029		14.20	A
50	ATOM	710	CG			156	51.603	11.273	-5.449		17.29	A
				TYR			52.857	11.429	-6.045		16.46	A
	ATOM	711							-7.360		18.68	A
	ATOM	712		TYR			52.978	11.884				A
26	ATOM	713		TYR			50.474	11.588	-6.202		16.43	
35	ATOM	714		TYR			50.583	12.048	-7.512		16.31	A
	ATOM	715	CZ			156	51.835	12.192	-8.083		18.17	A
	ATOM	716	ОН			156	51.941	12.651	-9.371		17.47	A
	ATOM	717	C			156	51.657	11.108	-1.572		16.32	A
	ATOM	718	0			156	52.412	10.197	-1.235		16.27	A
40	ATOM	719	N			157	50.678	11.568	-0.792		15.47	A
	ATOM	720	CA			157	50.385	10.966	0.508		16.66	A
	ATOM	721	CB			157	50.324	12.014	1.629		16.91	A
	ATOM	722	CG			157	51.631	12.708	1.907		18.96	A
	ATOM	723		PHE			52.821	12.261	1.340		20.31	A
45	MOTA	724	CD2	PHE	Α	157	51.664	13.829	2.732	1.00	21.12	A
	ATOM	725	CE1	PHE	Α	157	54.025	12.926	1.585	1.00	22.08	A
	MOTA	726	CE2	PHE	Α	157	52.865	14.500	2.982	1.00	22.18	A
	MOTA	727	CZ	PHE	Α	157	54.045	14.045	2.405	1.00	21.27	A
	ATOM	728	С	PHE	A	157	49.016	10.308	0.404	1.00	16.52	Α
50	ATOM	729	0	PHE	Α	157	48.029	10.979	0.110	1.00	17.32	A
	ATOM	730	·N	GLY	Α	158	48.953	9.002	0.644	1.00	15.97	A
	ATOM	731	CA			158	47.684	8.299			16.13	A
	ATOM	732	C			158	47.000	8.383	1.920		14.94	A
	ATOM ·	733	Ö			158	47.445	7.756	2.879		16.28	A
55	ATOM	734	N			159	45.915	9.145			13.50	A
	MOTA	735	CA			159	45.191	9.340			15.20	A
	MOTA	736	CB			159	45.031	10.835	3.517		14.20	A
	ATOM	737	CG			159	46.270	11.726			19.00	A
	ATOM	738		LEU			45.847	13.188			17.12	A
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	ATOM	739	CD2	LEU	A	159		47.275	11.390	4.471	1.00 14.71	A
	ATOM	740	C	LEU	A	159		43.809	8.716	3.232	1.00 15.53	A
	ATOM	741	0	LEU	A	159		43.232	8.472	2.177	1.00 16.05	A
	ATOM	742	N	SER	A	160		43.268	8.469	4.418	1.00 15.86	A
5	ATOM	743	CA	SER	Α	160		41.932	7.917	4.498	1.00 19.01	A
	ATOM	744	CB	SER	A	160		41.566	7.582	5.949	1.00 22.90	A
	ATOM	745	OG	SER	A	160		41.901	8.629	6.833	1.00 24.18	A
	ATOM	746	C	SER	Α	160		40.987	`.8.968	3.924	1.00 20.43	A
	ATOM	747	0	SER	Α	160		41.213	10.173	4.062	1.00 19.96	A
10	ATOM	748	N	TYR	A	161		39.945	8.508	3.250	1.00 19.20	A
	ATOM	749	CA	TYR	Α	161		38.975	9.406	2.644	1.00 20.37	A
	ATOM	750	CB	TYR	Α	161		38.471	8.785	1.332	1.00 20.00	A
	ATOM	751	CG	TYR	A	161		37.314	9.502	0.666	1.00 20.72	A
	ATOM	752	CD1	TYR	Α	161		37.222	10.895	0.682	1.00 18.22	A
15	ATOM	753	CE1	TYR	Α	161		36.180	11.557	0.029	1.00 22.24	A
	ATOM	754	CD2	TYR	A	161		36.333	8.784	-0.020	1.00 20.53	A
	ATOM	755	CE2	TYR	Α	161		35.287	9,436	-0.678	1.00 24.24	A
	ATOM	756	CZ	TYR	A	161		35.218	10.822	-0.648	1.00 22.32	Α
	ATOM	757	OH	TYR	A	161		34.194	11.471	-1.298	1.00 23.03	A
20	MOTA	758	C	TYR	Α	161		37.812	9.681	3.598	1.00 20.14	A
	ATOM	759	0	TYR	A	161		36.959	8.819	3.810	1.00 19.53	A
	ATOM	760	N	ALA	A	162		37.791	10.880/	4.178	1.00 19.92	A
	ATOM	761	CA	ALA	A	162		36.721	11.271	5.099	1.00 21.07	A
	MOTA	762	CB	ALA	A	162		37.187	12.419	6.002	1.00 19.60	A
25	MOTA	763	C	ALA	A	162		35.542	11.712	4.238	1.00 22.07	A
	MOTA	764	0	ALA	A	162		35.436	12.875	3.860	1.00 20.66	Α
	ATOM	765	N	LYS	Α	163		34.653	10.769	3.945	1.00 23.27	A
	MOTA	766	CA	LYS	Ą	163		33.503	11.017	3.080	1.00 27.12	A
	ATOM	767	CB	LYS	Α	163	-	32.663	9.741	2.963	1.00 29.68	A
30	ATOM	768	CG	LYS	Α	163		33.455	8.524	2.515	1.00 37.67	A
	MOTA	769	CD	LYS	A	163		32.556	7.310	2.321	1.00 42.24	A
	MOTA	770	CE	LYS	Α	163		33.373	6.034	2.185	1.00 44.48	A
	MOTA	771	NZ	LYS	A	163		34.143		. 3.430	1.00 44.88	· A
	ATOM	772	C	$rac{1}{1}$				32.581	12.186	3.411	1.00 25.78	A
35	ATOM	773	0	LYS				32.103	12.863	2.506	1.00 26.53	A
	MOTA	774	И.	ASN				32.327	12.441	4.689	1.00 24.57	A
	MOTA	775	CA	ASN				31.420	13.522	5.033	1.00 23.77	A
-	ATOM	776	CB	ASN				30.610	13.129	6.265	1.00 25.02	A
	ATOM	777	CG	ASN				29.537	12.101	5.932	1.00 27.54	A
40	MOTA	778		ASN				28.772	12.281	4.983	1.00 28.79	A
	MOTA	779		ASN			•	29.475	11.024	6.704	1.00 27.13	A
	MOTA	780	C	ASN				31.999	14.931	5.169	1.00 24.43	. A
	MOTA	781	0	ASN				31.306		~ 5.589	1.00 23.98	A
	ATOM	782	N .	GLY				33.262	15.097	4.795	1.00 21.56	A A
45	MOTA	783	CA	GLY				33.873	16.414	4.836	1.00 24.39	A
	MOTA	784	C	GLY				34.191	17.043	6.181	1.00 23.62	A A
	MOTA	785	0	GLY				34.380	16.352	7.177	1.00 23.26	A
	ATOM	786	N	GLU				34.234	18.373	6.186	1.00 23.22	A A
	ATOM	787				166		34.563	19.176	7.362	1.00 24.54	A
50	MOTA	788	CB	GLU				35.055	20.558	6.913	1.00 25.04	
	ATOM	789	CG	GLU				36.419	20.569	6.229	1.00 26.48 1.00 30.02	A A
	ATOM	790	CD			166		36.699	21.889	5.517		A
	ATOM	791		GLÜ				36.081	22.906	5.889	1.00 29.33 1.00 30.48	A
	ATOM	792		GLU				37.544	21.916	4.596	1.00 30.48	A
55	ATOM	793	C			166		33.436 32.279	19.372 19.541	8.369	1.00 24.44	A
	ATOM	794	0			166			19.341	8.001	1.00 22.76	A
•	ATOM	795	N			167		33.791	19.570	9.649	1.00 22.35	A
	ATOM	796	CA			167		32.813	19.581	10.707	1.00 22.28	A
	MOTA	797	CB	LEU	A	167		33.497	13.401	12.073	1.00 22.32	- 11

	ATOM	798	CG	LEU	Α	167		32.706	19.923	13.306	1.00	22.04	A
	MOTA	799	CD1	LEU	Α	167		31.454	19.074	13.463	1.00	19.66	A
	ATOM	800	CD2	LEU	Α	167		33.597	19.805	14.537	1.00	21.17	A
	ATOM	801	С	LEU	A	167		32.193	20.971	10.529	1.00	23.49	A
5	ATOM	802	0	LEU	Α	167		31.047	21.209	10.907	1.00	23.56	A
	ATOM	803	N	LEU	Α	168		32.960	21.887	9.948	1.00	24.25	A
	ATOM	804	CA	LEU				32.473	23.245	9.722	1.00	26.64	A
	ATOM	805	CB	LEU				33.560	24.099	9.066		25.62	A
	ATOM	806	CG	LEU				33.198	25.546	8.707		27.34	A
10	ATOM	807		LEU				32.718	26.296	9.946		26.42	A
10	ATOM	. 808		LEU				34.418	26.238	8.119		26.74	A
	ATOM	809	C	LEU				31.234	23.218	8.829		27.13	A
	ATOM	810	0	LEU				30.297	23.989	9.030		26.01	A
	ATOM	811	И	LYS				31.233	22.320	7.848		26.41	A
15		812	CA	LYS				30.106	22.320	6.934		27.70	A
13	ATOM		CB	LYS						5.945		30.49	· A
	ATOM	813						30.324	21.064			32.47	A
	ATOM	814	CG	LYS				29.151	20.854	4.993			A
	ATOM	815	CD	LYS				29.407	19.728	3.998		35.98	
00	ATOM	816	CE	LYS				29.462	18.372	4.683		38.53	A
20	ATOM	817	NZ	LYS				29.622	17.263	3.702		41.00	A
	ATOM	818	C	LYS				28.801	21.985	7.682		28.12	A
	ATOM	819	0	LYS			,	27.785	22.608	7.371		28.08	A
	ATOM	820	N	TYR				28.826	21.094	8.668		26.53	A
	ATOM	821	CA	TYR				27.624	20.791	9.434		26.95	A
25	ATOM	822	CB	TYR			-	27.810	19.476	10.193		25.03	A
	MOTA	823	CG	TYR				27.898	18.300	9.251		26.65	A
	MOTA	824		TYR				26.745	17.661	8.790		28.27	Α
	ATOM	825		TYR				26.814	16.642	7.839		26.85	A
	ATOM	826	CD2	TYR	A	170		29.127	17.884	8.742		27.83	A
30	ATOM	827	CE2	TYR				29.209	16.869	7.792		27.19	Α
	ATOM	828	CZ	TYR	A	170		28.049	16.254	7.343	1.00	30.02	A
	ATOM	829	OH	TYR	Α	170		28.130	15.268	6.382	1.00	29.23	A
	ATOM	830	C	TYR				27.229	21.918	10.376	1.00	27.59	A
	MOTA	831	0	TYR	A	170		26.045	22.122	10.642	1.00	29.25	A
35	ATOM	832	N	ILE	Α	171		28.208	22.660	10.882	1.00	28.16	A
	ATOM	833	CA	ILE	A	171		27.883	23.770	11.763	1.00	29.03	A
	ATOM	834	CB	ILE	A	171		29.151	24.435	12.337	1.00	27.51	A
	MOTA	835	CG2	ILE	Ą	171		28.773	25.705	13.084	1.00	27.97	A
	MOTA	836	CG1	ILE	Α	171		29.872	23.458	13.272	1.00	26.70	A
40	MOTA	837	CD1	ILE	Α	171		31.163	23.996	13.856	1.00	24.07	A
	MOTA	838	C	ILE	Α	171		27.094	24.796	10.944	1.00	31.41	Α
	ATOM	839	0	ILE	Α	171		26.088	25.335	11.407	1.00	31.69	A
	MOTA	840	N	ARG	Ą	172		27.546	25.047	9.719	1.00	33.21	Α
	MOTA	841	CA	ARG	Α	172		26.874	26.000	8.844	1.00	36.54	A
45	ATOM	842	CB	ARG	Α	172		27.734	26.314	7.616	1.00	37.73	A
	MOTA	843	CG	ARG	Α	172		29.057	27.011	7.912	1.00	41.65	A
	ATOM	844	CD	ARG	Α	172		29.708	27.492	6.616	1.00	45.29	A
	ATOM	845	NE	ARG	A	172		31.037	28.070	6.812	1.00	48.51	A
	ATOM	846	CZ	ARG				31.314	29.059	7.658	1.00	51.53	A
50	ATOM	847	NH1	ARG	Α	172		30.355	29.593	8.406	1.00	53.75	A
	MOTA	848	NH2	ARG	Α	172		32.553	29.526	7,748	.1.00	51.21	Α
	MOTA	849	С	ARG	Α	172		25.528	25.459	8.378	1.00	37.67	A
	ATOM	850	0	ARG				24.550	26.200	8.288	1.00	39.09	A
	ATOM	851	N	LYS				25.481	24.163	8.092	1.00	38.44	A
55	ATOM	852	CA	LYS				24.259	23.528	7.619	1.00	39.25	A
	ATOM	853	CB	LYS				24.523	22.061	7.272	1.00	41.89	· A
	MOTA	854	CG	LYS	Α	173		23.279	21.298	6.830		45.52	A
	MOTA	855	CD	LYS				23.557	19.808	6.653	1.00	49.60	A
	ATOM	856	CE	LYS				24.477	19.530	5.469		52.63	A

	ATOM	857	NZ	LYS	A	173	2	3.855	1.	9.894	4.160		0 54.		A
	ATOM	858	C	LYS	Α	173	. 2	3.089		3.608	8.595		0 39.		A
	MOTA	859	0	LYS	А	173	2	1.981		3.960	8.201		0 39.		A
	MOTA	860	N	ILE	Α	174		3.320		3.282	9.863		00 37.		A
5	MOTA	861	CA	ILE				2.229		3.314	10.833		00 37.		A
	MOTA	862	CB	ILE	A	174		2.159		1.998	11.652		00 37.4		A
	MOTA	863	CG2	ILE	Α	174		2.058		0.802	10.709		00 38.		A
	MOTA	864		ILE				23.397		1.850	12.532		00 37.		A
	MOTA	865	CD1	ILE				23.355		0.620	13.418		00 36.		. A
10	MOTA	866	C	ILE				22.259		4.492	11.801		00 36.		A
	MOTA	867	0	ILE				21.448		4.556	12.724		00 38.		A
	ATOM	868	N	GLY				23.185		5.423	11.592		00 35.		A
	ATOM	869	CA	GLY				23.265			12.462		00 35.		A
	ATOM	870	С	GLY				24.053		6.360	13.737		00 35.		A
15	ATOM	871	0	GLY				25.066		7.019	13.970		00 37.		A
	MOTA	872	N	SER				23.581		5.441	14.57		00 33.		A
	MOTA	873	CA	SER				24.253		5.113	15.822		00.32.		A
	MOTA	874	CB	SER				23.938		6.155	16.901		00 33.		A A
	MOTA	875	OG	SER				22.599		6.056	17.347		00 34.		A
20	MOTA	876	C	SER				23.796		3.731	16.276		00 32.		
	MOTA	<i>-</i> 877	0	SER				22.726		3.263	15.884		00 32.		A
	MOTA	878	N	PHE				24.609		3.085			00 29.		A A
	MOTA	879	CA	PHE				24.313		1.743	17.597		00 27.		
	MOTA	880	CB	PHE				25.621		0.989	17.869		00 26. 00 26.		A A
25	ATOM	881	CG	PHE				26.372		0.585	16.622		00 25.		A
	ATOM	882		PHE				26.210		1.277	15.426		00 25. 00 26.		A
	ATOM	883		PHE				27.266		9.516	16.662 14.290		00 26. 00 26.		Ā
	ATOM	884		PHE				26.923		0.912	15.532		00 26. 00 26.		A
20	ATOM	885		PHE				27.986		9.143	14.34		00 20. 00 25.		. A
30	ATOM	886	CZ			177		27.815		9.841	18.884		00 23. 00 27.		A
	MOTA	887	C			177		23.500 23.704		1.752 2.610	19.74		00 27. 00 26.		A
	MOTA	888	N O	ASP		177		22.578		0.802	19.02		00 26. 00 26.		A
	MOTA	889				178		21.816		0.729	20.26		00 26.		A
25	MOTA	890 891	CA CB			178		20.621		9.773	20.14		00 29.		A
35	MOTA	892	CG			178		21.020		8.372	19.72		00 32.		A
	ATOM ATOM	893		ASP				22.157		7.949	20.01		00 35.		A
	ATOM	894		ASP				20.179		7.683	19.10		00 34.		A
	MOTA	895	C			178		22.810		0.228	21.31		00 25.		A
40	ATOM	896	ō			178		23.974		9.968	20.99		00 21.		A
40	ATOM	897	N			179		22.361		0.083	22.55		00 23.		Α
	ATOM	898	CA			179		23.247		9.644	23.61		00 25.		. A
	ATOM	899	CB			179		22.542		9.770	24.97		00 27.		A
	ATOM	900	CG			179		23.324		9.176	26.13		00 32.	58	A
45	ATOM	901	CD			179		22.997		9.845	27.44		00 35.	82	A
73	ATOM	902		GLU				21.825		0.224	27.64		00 35.		A
	ATOM	903		GLU				23.912		9.984	28.29		00 38.		A
	ATOM	904	C			179		23.808		8.235	23.45		00 24.		A
	ATOM	905	ō	GLU				24.977		7.989	23.75		00 22.	79	A
50	ATOM	906	N			180		22.983		7.316	22.96		00 23.	36	A
	ATOM	907	CA			180		23.412		5.935	22.76	1 1.	00 22.	15	Α
	MOTA	908	CB			180		22.224		5.054	22.32		00 23.	77	A
	ATOM	909		THR				21.222		5.075	23.34	1 1.	00 26.	37	Α
	ATOM	910		THR				22.670		3.616	22.08		00 22.		A
55	ATOM	911	C			180	:	24.533		5.830	21.72		00 22.		A
-	ATOM	912	0	THR	Α	180	:	25533	. 1	5.141	21.94		00 19.		A
	MOTA	913	N	CYS	Α	181	:	24.365	1	6.511	20.59		00 21.		A
	ATOM	914	CA			181		25.372	: 1	6.480	19.54		00 22.		A
	MOTA	915	CB	CYS	A	181		24.800) 1	7.065	18.25	0 1.	00 24.	62	A

	ATOM	916	SG	CYS 2	A	181		23.	435		080	17.	560	1.0	0	29.50	7	Ā
	ATOM	917	C	CYS 2	A	181	•	26.	633	17.	232		954	1.0	0	23.07	1	Ą
	ATOM	918	0	CYS 2	A.	181		27.	746	16.	827	19.	608	1.0	00	23.95	7	J.
	ATOM	919	N	THR .	A	182		26.	463	18.	325	20.	695	1.0	00	22.76	7	4
5	ATOM	920	CA	THR .	A	182		27.	606	19.	103	21.	161	1.0	0 0	21.49	7	ð.
	ATOM	921	CB	THR .	A	182		27.	167	20.	346		978	1.0	00	21.37		4
	ATOM	922	OG1	THR .	Ą	182		26.	459	21.	262	21.	134	1.0	00	22.50	` 1	4
	A'TOM	923	CG2	THR .	A	182		28.	379	21.	046	22.	565	1.0	00	18.36	1	4
•	ATOM	924	C	THR .	Α	182		28.	454	18.	215	22.	071	1.0	0.0	21.48	7	Ą
10	MOTA	925	0	THR .	A	182		29.	669	18.	090	21.	894			19.95	1	7
	ATOM	926	N	ARG .	Α	183		27.	.798	17.	602	23.	050	1.0	0 0	18.97	ì	A
	ATOM	927	CA	ARG .	A	183		28.	468	16.	723	23.	996	1.0	00	19.39	1	Ą
	ATOM	928	CB	ARG .	A	183		27.	. 455	16.	140	24.	.984			19.46		Α.
	ATOM	929	CG	ARG .	Ą	183		28.	.030	15.	062	25.	887			18.77	. 1	A.
15	ATOM	930	CD	ARG .	Α	183		27.	.021	14.	571	26.	925			21.19		Ą
	ATOM	931	NE	ARG .	A	183		26.	. 605	15.	642	27.	824			19.46		A
	MOTA	932	\mathbf{cz}	ARG .	Α	183		25.	. 496	16.	362	27.	679			20.45		A
	ATOM	933	NH1	ARG	A.	183		24.	672	16.	123	26.	. 666	1.0	00	19.81	1	A.
	MOTA	934	NH2	ARG	A	183		25	. 224	17.	338	28.	. 539	1.0	00	17.11		A.
20	ATOM	935	C	ARG	A	183		29	.206	15.	577	23.	.302			20.02	i	A
	MOTA	936	0	ARG	Α	183		30.	. 383	15.	333	23	. 573	1.0	00	19.97	1	A
	MOTA	937	N	PHE	Α	184		28	.520	14.	871	22	.409	1.	00	19.24	7	A
	MOTA	938	CA	PHE	Α	184		29	.144	13.	746	21.	.722	1.	00	18.04	3	A
	MOTA	939	CB	PHE	Α	184		28	.158	13.	078	20	.764	1.0	00	21.05	1	A
25	ATOM	940	CG	PHE	Α	184		28	.719	11.	857		.098	1.	00	22.67	j	A
	ATOM	941	CD1	PHE	A	184		28	.717	10.	630	20	.754			22.97		A
	ATOM	942	CD2	PHE	Α	184		29	.317	11.	949	18	.850	1.	00	19.97		A
	ATOM	943	CE1	PHE	Α	184		29	.308	9.	510	20	.176	1.	00	23.53	2	A
	ATOM	944	CE2	PHE	Α	184		29	.915	10.	. 833	18	.263	1.	00	24.11		A,
30	ATOM	945	CZ	PHE	Α	184		29	.910	9.	613	18	. 928	1.	00	22.97		A
	MOTA	946	C	PHE	A	184		30	.403	14.	. 127	20	.941			17.99		A
	MOTA	947	0	PHE	Α	184		31	.461	13.	.531	21	.130	1.	00	18.89		A
	MOTA	948	N	TYR	Α	185		30	.292	15.	.110	20	.056			15.73		A
	ATOM	949	CA	TYR	A	185		31	.443	15	.519		.265			15.72		A
35	MOTA	950	CB	TYR	Α	185		30	.992	16.	. 413	18	.111			17.33		A
	ATOM	951	CG	TYR	Α	185		30	.364	15	.584 [,]	17	.015			19.37		A
	MOTA	952	CD1	TYR	Α	185		31	.159	14	. 809	16	.168			16.53		A
	MOTA	953	CE1	TYR	Α	185		30	.590	13.	. 952		.232			18.12		A.
	MOTA	954	CD2	TYR	Α	185		28	.976	15	.484		.892			18.18		A
40	ATOM	955	CE2	TYR	Α	185		28	.398		623		.956			18.90		A
	ATOM	956	CZ	TYR	A	185		29	.211	13	861		.133			18.41		A.
	MOTA	957	ОН	TYR					.650		. 995		.218			20.48		A
	ATOM	958	C	TYR	Α	185			.544		.172		.083			15.79		A
	ATOM	959	0	TYR					.720		.015		.766			17.69		A
45	ATOM	960	N	THR					.176		.887		.142			15.68		A
	ATOM	961	CA	THR					.184		.504		. 997			16.03		A
	MOTA	962	CB	THR					.559		.403		.094			16.62		A
	ATOM	963		THR				31	.866		.503		.481			14.79		A
	MOTA	964	CG2	THR					.656		.953		.019			14.68		A
50	MOTA	965	C	THR					.954		.375		.680			15.59		A
	MOTA	966	0	THR					.176		.443		.823			13.77		A
	MOTA	967	N	ALA					.234		.333		.097			14.06		A
	MOTA	968	CA	ALA					.869		.196		.757			14.74		A
	ATOM	969	CB	ALA					.810		.195		.224			14.32		A
55	ATOM	970	C	ALA					.875		.509		.821			14.41		A
	MOTA	971	0	ALA					.972		.136		.247			15.61		A
	MOTA	972	N	GLU					.516		.340		.549			14.01		A
	MOTA	973	CA	GLU					.443		.704		.615			13.50		A
	MOTA	974	CB	\mathtt{GLU}	Α	188	•	34	.782	12	.449	19	.251	1.	00	12.85		А

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	ATOM	975	CG	GLU	A	188	3.	3.622	:	11.454	19.282	1.00	12.71	A
	MOTA	976	CD	GLU	A	188	3	3.464	:	10.685	17.979		15.01	A
	ATOM	977	OE1	GLU	Α	188	3	3.687	' ;	11.275	16.899	1.00	13.21	A
	ATOM	978	OE2	GLU	Α	188	3	3.110)	9.484	18.031	1.00	17.69	A
5	ATOM	979	C	GLU	Α	188	3	6.682	: :	13.582	20.436	1.00	13.34	A
	MOTA	980	0	GLU	Α	188	3	7.803	. :	13.085	20.408	1.00	14.69	A
	ATOM	981	N	ILE	Α	189	3	6.486	;	14.893	20.326	1.00	13.52	A
	ATOM	982	CA	ILE	Α	189	3	7.627	,	15.787	20.159	1.00	13.35	A
	ATOM	983	CB	ILE	Α	189	3	7.169)	17.247	19.939	1.00	13.95	A
10	ATOM	984	CG2					8.381		18.165	19.822	1.00	12.47	A
- •	MOTA	985		ILE			3	6.302	:	17.332	18.671	1.00	13.44	A
	MOTA	986		ILE				5.588		18.664	18.491	1.00	14.29	A
	MOTA	987	С	ILE	Α	189		8.530		15.702	21.394	1.00	14.63	A
	ATOM	988	0			189		9.753		15.595	21.271	1.00	12.97	A
15	MOTA	989	N			190		7.927		15.751	22.582	1.00	14.35	A
13	ATOM	990	CA			190		8.684		15.655	23.832	1.00	13.22	Α
	ATOM	991	CB			190		7.743		15.690	25.061	1.00	14.28	A
	ATOM	992		VAL				8.509		15.267	26.326		15.08	. A
	ATOM	993		VAL				7.160		17.082	25.233		12.08	A
20	ATOM	994	C			190		9.468		14.338	23.859		14.61	A
20	ATOM	995	o			190		0.634		14.304	24.250		13.72	A
		996	N			191		8.825		13.254	23.432		15.26	A
	ATOM ATOM	997				191		9.478		11.943	23.421		16.81	A
		998	CB			191		8.470		10.857	23.041		16.14	A
25	ATOM	999	OG			191		9.018		9.569	23.238		16.94	A
23	MOTA MOTA	1000	C			191		0.649		11.928	22.441		16.58	A
	ATOM	1001	Ö			191		1.697		11.335	22.713		13.96	A
	MOTA	1001	N			192		0.468		12.586	21.300		15.26	A
	ATOM	1003	CA			192		1.518		12.645	20.292	1.00	14.37	A
30	ATOM	1004	CB			192				13.296	19.016	1.00	14.43	A
50	MOTA	1005	C.			192		2.695		13.440	20.845	1.00	16.46	A
	ATOM	1005	ō			192		3.851		13.038	20.697	1.00	17.96	A
	ATOM	1007	N			193		2.401		14.563	21.496	1.00	15.02	A
	ATOM	1008	CA			193		3.459		15.392	22.067	1.00	15.42	A
35	ATOM	1009	CB			193		2.884		16.712	22.600	1.00	12.88	A
55	ATOM	1010	CG			193		2.445		17.721	21.525	1.00	15.97	A
	ATOM	1011		LEU			•	1.869		18.979	22.190	1.00	13.97	, A
	MOTA	1012		LEU				3.642		18.088	20.655	1.00	14.58	A
	ATOM	1013	C			193	. 4	4.211	1	14.659	23.174	1.00	14.49	. A
40	ATOM	1014	ō			193		5.427		14.813	23.310	1.00	16.56	Α
	MOTA	1015	N			194		3.500		13.870	23.975	1.00	13.96	A
	ATOM	1016	CA			194		4.179		13.123	25.032	1.00	14.08	А
	ATOM	1017	CB			194	4	3.190	0	12.295	25.857	1.00	14.65	A
	ATOM	1018	CG			194		3.882		11.301	26.789	1.00	17.09	A
45	ATOM	1019	CD			194	4	2.924	4	10.592	27.730	1.00	19.59	A
73	ATOM	1020		GLU				1.809		10.237	27.295		19.25	A
	ATOM	1021		GLU				3.302		10.380	28.906	1.00	20.20	A
	ATOM	1022	C			194		5.208		12.199	24.386	1.00	13.57	A
	ATOM	1023	ō			194		6.33		12.093	24.847		14.23	A
50	ATOM	1024	N			195		4.822		11.544	23.301	1.00	14.89	. A
••	ATOM	1025	CA			195	4	15.743	3	10.642	22.618	1.00	16.58	Α,
	ATOM	1026	CB			195		5.03		9.910	21.488	1.00	17.29	A
	ATOM	1027	CG			195		15.95		9.058	20.649		17.92	A
	ATOM	1028		TYR				16.34		7.788	21.077	1.00	17.96	A
55	ATOM	1029		TYR				17.20		6.996	20.304		19.77	A
55	ATOM	1030		TYR				16.44		9.524	19.428	1.00	16.67	A
	ATOM	1031		TYR				17.29		8.744	18.650		18.51	A
	ATOM	1032	CZ			195	4	17.67	1	7.481	19.094	1.00	20.24	A
	ATOM	1033	OH			195	4	18.50	6	6.705	18.325	1.00	21.89	A

	MOTA	1034	С	TYR	A	195	46.	.917	11.419	22.035	16.98	A
	ATOM	1035	0	TYR	Α	195	48.	.081	11.047	22.203	14.61	A
	MOTA	1036	N	LEU	Α	196	46.	.599	12.507	21.347	16.30	A
	MOTA	1037	CA	LEU	A	196	47.	.619	13.328	20.720	18.15	A
5	MOTA	1038	CB	LEU	Α	196	46	. 969	14.502	19.982	18.59	A
	MOTA	1039	CG	LEU	Α	196	47.	.834	15.203	18.935	22.51	A
	MOTA	1040	CD1	LEU	Α	196	48.	.222	14.206	17.841	 20.94	A
	MOTA	1041	CD2	LEU	Α	196	47	.060	16.375	18.338	22.98	A
	MOTA	1042	C	LEU	Α	196	48	.592	13.844	21.763	17.75	Α
10	MOTA	1043	0	LEU	Α	196	49	.801	13.644	21.649	18.33	A
	MOTA	1044	N	HIS	Α	197	48	.064	14.495	22.792	17.12	A
	ATOM	1045	CA	HIS	A	197	48	.913	15.042	23.842	18.47	A
	MOTA	1046	CB	HIS	A	197	48	.069	15.866	24.817	15.90	A
	MOTA	1047	CG	HIS	A	197	47	.571	17.152	24.231	19.15	A
15	MOTA	1048	CD2	HIS	A	197	47	.830	17.745	23.038	18.22	A
	MOTA	1049		HIS			46	.704	17.992	24.897	17.47	A
	MOTA	1050		HIS		_	46	.450	19.047	24.139	19.74	A
	MOTA	1051	NE2	HIS	A	197	47	.119	18.921	23.007	15.69	A
	MOTA	1052	C			197		.696	13.958	24.572	19.40	A
20	MOTA	1053	0	HIS	Α	197	50	.823	14.192	25.021	19.42	A
	ATOM	1054	N	GLY	Α	198		.106	12.770	24.679	18.59	A
	ATOM	1055	CA	GLY	Α	198		.793	11.675	25.339	19.60	A
	ATOM	1056	C			198		.075	11.307	24.612	21.86	A
	ATOM	1057	0			198		.963	10.682	25.186	23.09	A
25	MOTA	1058	N			199		.174	11.687	23.341	22.81	· A
	ATOM	1059	CA			199		.368	11.401	22.549	24.43	A
	MOTA	1060	CB			199		.990	10.905	21.154	26.00	A
	ATOM	1061	CG			199		.378	9.520	21.133	30.98	A
	ATOM	1062	CD			199		.291	9.002	19.708	36.85	. A
30	MOTA	1063	CE			199		.832	7.559	19.682	40.37	A
	MOTA	1064	NZ			199		.646	6.691	20.581	43.48	A
	MOTA	1065	C			199		.253	12.631	22.414	23.88	A
	MOTA	1066	0			199		.144	12.669	21.568	24.97	A '
	MOTA	1067	N			200			13.638	23.243	24.00	A · A
35	MOTA	1068	CA			200		.790	14.853	23.203	22.12	A
	MOTA	1069	C			200		.665	15.632	21.907	22.14 22.41	A
	ATOM	1070	0			200		.632	16.231	21.439	20.00	A
	ATOM	1071	N			201		.475	15.630	21.320	18.93	A
	MOTA	1072	CA			201		.252	16.355	18.955	19.70	A
40	ATOM	1073	CB			201		.784	15.414	17.716	20.12	A
	ATOM	1074		ILE		•		.414	16.226	18.636	20.03	A
	MOTA	1075		. ILE				.880	14.395 13.258	17.745	22.75	A
	ATOM	1076		ILE		201		.408	17.425	20.270	19.87	A
	ATOM	1077	C			201		.121		20.817	20.08	A
45	MOTA	1078	0					.508	18.633	19.815	19.94	A
	MOTA	1079	N			202		.601	19.772	19.891	20.45	A
	MOTA	1080	CA			.202		.352		20.356	22.21	A
	АТОМ МОТА	1081 1082	CB	: ILE		202		.381	22.220	20.470	22.67	Α
50	ATOM	1082		ILE				.033	20.775	21.700	24.19	A
50		1084		ILE				.914	21.920	22.169	25.39	Α
	ATOM ATOM	1084	C			202		.105	19.999	18.464	20.71	A
	ATOM	1086	0			202		.910	20.067	17.538	19.48	A
	MOTA	1086	N			202		.795	20.108	18.270	18.65	A
55	MOTA	1088	CA			203		.280	20.319		18.02	A
22	ATOM	1089	CB			203		.775	20.057	16.874	16.31	Ä
	ATOM	1090	CG			203		.199	20.136	15.495	18.36	A
	ATOM	1091		HIS				.043	21.186	14.655	16.42	A
	ATOM	1092		L HIS				.759	19.026		19.50	A
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	ATOM	1093	CE1	HIS 2	A	203	45	.359	19.	389	13.60	0		17.64		A
	MOTA	1094	NE2	HIS 2	A	203	45	.522	20.	694	13.48	3		20.87		Α
	ATOM	1095	C	HIS 2	Α	203	48	.589	21.	738	16.40	5		18.92		A
	MOTA	1096	0	HIS 2	A	203	49	.073	21.	906	15.28			16.21		A
5	MOTA	1097	N	ARG 2	A	204	48	.301	22.	744	17.23	2		18.60		A
	ATOM	1098	CA	ARG 2	A	204	48	.552	24.	157	16.91			19.81		A
	MOTA	1099	CB	ARG 2	A	204	49	.998	24.	365	16.45			21.61		A
	ATOM	1100	CG	ARG .	A	204	51	.024	24.	137	17.55			23.82		Α
	MOTA	1101	CD	ARG .	Α	204	52	.323	24.	870	17.25			27.62		A
10	MOTA	1102	NE	ARG .				.932	24.		15.99			29.43		A
	MOTA	1103	CZ	ARG .	A	204	54	.125	24.	861	15.57			33.10		A
	MOTA	1104	NHl	ARG .	A	204	54	.835	25.	706	16.31			32.12		A
	MOTA	1105	NH2	ARG .	A	204	54	.614	24.	426	14.41			30.25	,	A
	MOTA	1106	С	ARG .			47	.624	24.	830	15.90			20.03		A
15	MOTA	1107	0	ARG .	A	204	47	.711	26.	038	15.69			20.88		A
	MOTA	1108	N	ASP .	A	205	46	.755		071	15.25			18.96		A
	MOTA	1109	CA	ASP	A	205	45	.828	24.	692	14.32			17.90		A
	MOTA	1110	CB	ASP .	A	205	46	.418		741	12.91			18.95		A
	MOTA	1111	CG	ASP				. 655		688	12.00			20.36		A
20	ATOM	1112		ASP				.939		560	12.54			20.35		A
	MOTA	1113	OD2	ASP	A	205	45	.772	25.	573	10.77			22.49		A
	.ATOM	1114	C	ASP	Α	205	44	.500		956	14.32			19.60		A
	MOTA	1115	0	ASP	Α	205	43	.876	23.	751	13.28			21.53		A
	ATOM .	1116	N	LEU	A	206	44	.063	23.	569	15.52			18.53		A
25	MOTA	1117	CA	LEU	A	206		.813		851	15.66			19.18	•	A
	ATOM	1118	CB	LEU	A	206	42	.693		295	17.08			18.94		, A
	MOTA	1119	CG	LEU	A	206	41	.511	21.	358	17.34			23.10		A
	MOTA	1120	CD1	LEU	A	206	41	.615		142	16.43			23.01		A
	MOTA	1121	CD2	TE Û	A	206	41	.504		933	18.80			22.97		A
30	ATOM	1122	С	TEU	A	206	41	.639		772	15.36			19.05		A
	ATOM	1123	0	LEU	A	206	41	.556		880	15.88			19.25		A
	ATOM	1124	N	LYS	Α	207	40	.740		307	14.50			17.54		A.
	MOTA	1125	CA	LYS	A	207	39	.564		081	14.11			18.60		A
	ATOM	1126	CB	LYS	Α	207	39	.980		248	13.19			18.98		A
35	ATOM	1127	CG	LYS	A	207	40	.786		817	11.98			18.20		A
	MOTA	1128	CD	LYS	Α	207		.246		000	11.13			21.42		A
	MOTA	1129	CE	LYS	Α	207	42	.223		537	10.06			23.21		A
	MOTA	1130	NZ	LYS	A	207		.561		604	9.08			29.61		A.
	MOTA	1131	C	LYS	Α	207		.566		181	13.38			18.18		A
40	MOTA	1132	0	LYS	A	207		.921		100	12.91			18.11		A
	MOTA	1133	N	PRO				.298		614	13.29			20.26		A
	MOTA	1134	CD	PRO				.713		833	13.88			18.79		A
	MOTA	1135	CA	PRO				.272		814	12.63			19.67	٠.	A
	MOTA	1136	CB			208		.063		742	12.60			19.45		A
45	MOTA	1137	CG	PRO				.231		509	13.89			21.81		A
	MOTA	1138	С	PRO				6.674		372	11.20			21.04		A
	MOTA	1139	0			208		.264		307	10.75			21.19		A
	MOTA	1140	N	GLU				474		188	10.52			21.69	•	A
	MOTA	1141	CA	GLU				.928		872	9.17			22.64		A
50	MOTA	1142	CB	GLU				3.644		.084	8.59			23.65		A
	MOTA	1143	CG	GLU				9.253		825	7.18			27.24	•	A
	MOTA	1144	CD			209		.155		. 958	6.7			29.40		A
	MOTA	1145		. GLU				9.660		.094	6.55			29.68		A
	MOTA	1146		GLU				L.363		.711	6.5			30.07		A.
55	MOTA	1147	C			209		3.879		.668	9.15			22.28		A
	MOTA	1148	0			209		3.955		. 933	8.1			21.36		Α
	MOTA	1149	N			210		.600		.490	10.20			19.90		A.
	MOTA	1150	CA			210).574		.412	10.43			19.44		A
	MOTA	1151	CB	ASN	A	210	4	1.744	20	.912	11.2	87	1.00	20.07		A

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	ATOM	1152	CG	ASN A	210		42.746	21.698	10.479	1.00 25.77	A
	ATOM	1153		ASN A			43.571	22.427	11.029	1.00 26.73	A
	ATOM	1154		ASN A			42.687	21.548	9.158	1.00 25.15	Α
	ATOM	1155	С	ASN A	210		40.005	19.151	11.078	1.00 18.63	Α
5	ATOM	1156	0	ASN A	210		40.712	18.154	11.234	1.00 18.29	A
-	ATOM	1157	N	ILE A	211		38.739	19.202	11.469	1.00 16.31	A
	MOTA	1158	CA	ILE A	211		38.090	18.058	12.085	1.00 15.49	A.
	MOTA	1159	CB	ILE A	211		37.336	18.488	13.354	1.00 15.40	A
	MOTA	1160	CG2	ILE A	211		36.582	17.311	13.950	1.00 14.59	A
10	MOTA	1161	CG1	ILE A	211		38.342	19.046	14.365	1.00 15.91	A
	ATOM	1162	CD1	ILE A	211		37.720	19.669	15.590	1.00 15.98	A
	MOTA	1163	C	ILE A	211		37.131	17.485	11.059	1.00 17.26	A
	ATOM	1164	0	ILE A	211		35.995	17.947	10.926	1.00 18.16	A
	ATOM	1165	N	LEU A	212		37.599	16.486	10.317	1.00 15.97	A
15	MOTA	1166	CA	LEU A	212		36.784	15.875	9.274	1.00 17.08	Α
	ATOM	1167	CB	LEU A	212		37.685	15.249	8.202	1.00 17.78	A
	MOTA	1168	CG	LEU A			38.785	16.157	7.640	1.00 18.92	A
	MOTA	1169	CD1	LEU A			39.476	15.450	6.485	1.00 22.09	A
	MOTA	1170	CD2				38.188	17.482	7.166	1.00 19.91	. A
20	MOTA	1171	С	LEU A			35.843	14.825	9.837	1.00 18.35	A
	MOTA	1172	0	LEU A			35.957	14.433	11.002	1.00 19.39	A A
	MOTA	1173	N	LEU A			34.915	14.368	9.000	1.00 17.84	A
	MOTA	1174	CA	LEU A			33.942	13.362	9.403	1.00 19.94	A
	ATOM	1175	CB	LEU A			32.556	14.004	9.487	1.00 20.84 1.00 20.31	A
25	MOTA	1176	CG	LEU A			32.396	15.059	10.583	1.00 20.31	A
	MOTA	1177		LEU A			31.124	15.837	10.367 11.940	1.00 22.73	À
	ATOM	1178		LEU A			32.379	14.378	8.426	1.00 20.98	A
	ATOM	1179	C	LEU A			33.914	12.187 12.379	7.218	1.00 20.55	. A
	MOTA	1180	0	LEU A			33.743	10.970	8.935	1.00 20.44	A
30	ATOM	1181	N	ASN A			34.088 34.055	9.814	8.049	1.00 23.77	Α
	ATOM	1182	CA	ASN A			34.745	8.596	8.674	1.00 25.30	A
	ATOM	1183	CB	ASN A			34.077	8.127	9.948	1.00 32.04	A
	ATOM	1184	CG	ASN F			32.908	8.422	10.206	1.00 34.43	Α
25	ATOM	1185 1186		ASN F			34.818	7.369	10.752	1.00 33.85	. A
35	MOTA MOTA	1187	C	ASN A			32.618	9.466	7.693	1.00 24.07	A
	ATOM	1188	,c O	ASN A			31.672	10.113	8.150	1.00 19.94	A
	ATOM	1189	N	GLU A			32.459	8.433	6.879	1.00 25.77	A
	ATOM	1190	CA	GLU 2			31.138	8.003	6.445	1.00 28.69	· A
40	ATOM	1191	CB	GLU A			31.275	6.796	5.513	1.00 31.98	Ä
40	ATOM	1192	CG	GLU A			29.970	6.334	4.896	1.00 40.22	A
	ATOM	1193	CD	GLU A			30.182	5.312	3.795	1.00 44.27	Α
	ATOM	1194		GLU A			30.817	4.268	4.065	1.00 46.46	Α
	ATOM	1195	OE2				29.716	5.556	2.660	1.00 46.13	A
45	ATOM	1196	· C	GLU A	A 215		30.188	7.673	7.601	1.00 28.41	, A
	ATOM	1197	0	GLU A			28.971	7.769	7.447	1.00 28.52	A
	ATOM	1198	N	ASP A	A 216		30.737	7.287	8.752	1.00 26.77	Α
	ATOM	1199	CA	ASP A			29.914	6.953	9.917	1.00 27.28	A
	ATOM	1200	CB	ASP A			30.538	5.795	10.696	1.00 31.27	A
50	MOTA	1201	CG	ASP A	A 216	;	30.390	4.466	9.979	1.00 37.61	A
	MOTA	1202	ODI	L ASP	A 216	5	29.274	4.170	9.499	1.00 39.45	A
	ATOM	1203	OD2	ASP A			31.382	3.710	9.902	1.00 41.84	A
	ATOM	1204	С	ASP 2			29.697	8.135	10.862	1.00.26.37	A
	ATOM	1205	0	ASP 2			29.136	7.984	11.950	1.00 25.73	A
55	MOTA	1206	N		A 217		30.156	9.306	10.441	1.00 23.02	A
	MOTA	1207	CA		A 217		30.015	10.527	11.218	1.00 21.83	A A
	MOTA	1208	CB		A 217		28.537	10.789	11.517	1.00 23.24	A A
	MOTA		CG		A 217		27.742	11.186	10.274	1.00 22.98	A A
	ATOM	1210	SD	MET	A 217	1	28.464	12.616	9.430	1.00 27.57	A

	ATOM	1211	CE	MET 2	A 2	217	27.	679	13.9	974	10.3		1.00	26.68	A
	ATOM	1212	С	MET 2	A 2	217	30.	844	10.0	518	12.5	502		21.51	A
	ATOM	1213	0	MET .	A 2	217	30.	474	11.3	323	13.4	140	1.00	18.62	A
	ATOM	1214	N	HIS !	A 2	218	31.	. 957		892	12.5	544		20.10	A
5	ATOM	1215	CA	HIS !	A 2	218	32.	873	9.	964	13.6	578		19.86	A
	MOTA	1216	CB	HIS .	A 2	218	33.	482	8 - 9	594	13.9	977		20.21	A
	ATOM	1217	CG	HIS .	A 2	218	32.	.551	7.	667	14.6	598		22.40	A
	MOTA	1218	CD2	HIS .	A 2	218	31.	.910	6.	547	14.2	287		21.27	A
	MOTA	1219	ND1	HIS .	A 2	218	32.	.177	7.	863	16.0			19.59	A
10	ATOM	1220	CE1	HIS .	A 2	218		.348		902	16.3			21.88	A
	ATOM	1221	NE2	HIS .	A 2	218		.168		091	15.3			22.08	A -
	ATOM	1222	C	HIS .	A 2	218	33	.947	10.		13.:			19.10	A
	MOTA	1223	0	HIS .	A 2	218	34	.170	11.		11.5			20.31	A
	ATOM	1224	N	ILE .			34	.617	11.		14.			17.21	A
15	MOTA	1225	CA	ILE .	A 2	219		.628	12.	586	13.0			15.26	A
	MOTA	1226	CB	ILE .	A 2	219		.987	13.		14.			15.38	A
	MOTA	1227	CG2					.722	14.		15.:			14.58	A
	MOTA	1228	CG1					.734	12.		15.			14.46	A
	MOTA	1229	CD1					.279	13.		16.			13.74	A
20	MOTA	1230	C	ILE				.929	11.		13.			16.21	A
	MOTA	1231	0	ILE				.238	10.		13.			15.88	. A
	MOTA	1232	N	GLN				.677	12.		12.			15.62	A
	MOTA	1233	CA	GLN				.980	12.		11.			17.84	·A
	MOTA	1234	CB	GLN				.872	11.		10.			20.00	A
25	MOTA	1235	CG	GLN				.463	10.		10.			26.97	A
	MOTA	1236	CD	GLN				.648		343		372		29.95	A
	ATOM	1237		GLN				.968		590		373		33.12	A
	ATOM	1238		GLN				.578		393		389		30.47	A
	ATOM	1239	C	GLN				.757	13.		11.) 17.00) 18.27	A
30	ATOM	1240	0	GLN				.609		339	10. 12.			14.34	A
	ATOM	1241	N	ILE				.566		906	12.			14.46	A
	ATOM	1242	CA	ILE				.361		120 416	14.			12.30	A
	ATOM	1243	CB	ILE				.867 .764		656	14.			14.78	
25	ATOM	1244	CG2	ILE				.660		613	15.			13.92	A
35	MOTA	1245						.003		901	16.			15.06	
	ATOM	1246	CD1	ILE				.536		996	11.			15.44	_
	MOTA	1247	0	ILE				.106		915	11.			13.93	Α
	ATOM	1248 1249	N.	THR				1877		101	11.			15.36	
40	ATOM ATOM	1249	CA	THR				.980		098	10.			17.52	_
40	ATOM	1251	CB	THR				.470		836		750		19.92	
	ATOM	1252	OG1					.587		637		875		18.78	
	MOTA	1253	CG2					.630		018		257		18.16	_
	ATOM	1254	C	THR				.735		428		192		19.60	
45	ATOM	1255	Ö	THR				.509		257		084	1.00	18.59	A
	ATOM	1256	N	ASP				.630		610		216		18.69	
	ATOM	1257	CA	ASP				.440		825		069		20.12	
	ATOM	1258	CB	ASP				.532		065		108	1.00	23.51	A
	ATOM	1259	CG	ASP				.248		335	8.	670	1.00	27.09	A
50	ATOM	1260		ASP				.283		227	7.	975	1.00	26.28	A
-	ATOM	1261		ASP				.765		438	9.	009	1.00	26.15	A
	ATOM	1262	·C	ASP				.516		913	10.	150		21.73	
	ATOM	1263	ō	ASP			47	.439	19.	751	11.	055	1.0	22.76	
	ATOM	1264	N	PHE				.535		063	10.	027		0 20.75	
55	ATOM	1265	CA	PHE			49	.611	17.	988	11.	009		0 20.11	
	MOTA	1266	CB	PHE	Α	224	49	.805	16.	527		424		0 20.62	
	ATOM	1267	CG	PHE			48	.682	15.	991	12.	263		0 21.41	
	ATOM	1268		PHE			48	.598		312		614		0 23.05	
	` ATOM	1269	CD2	PHE	Α	224	47	.681	15.	212	11.	693	1.0	0 22.27	A

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	ATOM	1270		PHE			47.528	15.868	14.389	1.00 23.30	A
	ATOM	1271	CE2	PHE	A	224	46.606	14.763	12.457	1.00 21.11	A
	ATOM	1272	CZ	PHE	A	224	. 46.530	15.093	13.807	1.00 22.02	A
	ATOM	1273	C	PHE			50.957	18.583	10.619	1.00 20.45	A
5	ATOM	1274	0	PHE	A	224	51.905	18.547	11.407	1.00 20.73	A
	ATOM	1275	N	GLY	A	225	51.049	19.125	9.412	1.00 22.02	A
	MOTA	1276	CA	GLY			52.301	19.713	8.981	1.00 22.66	A
	MOTA	1277	C	GLY	Α	225	52.742	20.822	9.920	1.00 24.99	A
	MOTA	1278	0	GLY	Α	225	53.939	21.041	10.122	1.00 24.52	A
10	ATOM	1279	N	THR	Α	226	51.779	21.524	10.508	1.00 23.50	A
	ATOM	1280	CA	THR	Α	226	52.106	22.613	11.416	1.00 25.16	Α
	MOTA	1281	CB	THR	Ą	226	51.199	23.829	11.160	1.00 24.76	A
	ATOM	1282	OG1	THR	Α	226	49.831	23.410	11.113	1.00 22.68	Α
	MOTA	1283	CG2	THR	A	226	51.571	24.490	9.834	1.00 25.00	A
15	MOTA	1284	С	THR	A	226	52.046	22.233	12.894	1.00 25.79	A
	MOTA	1285	0	THR	Α	226	52.019	23.100	13.768	1.00 24.54	A
	ATOM	1286	N	ALÁ	Α	227	52.037	20.935	13.173	1.00 24.97	A
	MOTA	1287	CA	ALA	A	227	52.004	20.475	14.550	1.00 25.49	A
	ATOM	1288	CB	ALA	Α	227	51.659	18.993	14.607	1.00 22.85	A
20	MOTA	1289	C	ALA	A	227	53.384	20.715	15.149	1.00 27.70	A
	ATOM	1290	0	ALA	Α	227	54.331	21.047	14.435	1.00 26.60	A
	MOTA	1291	N	LYS	Α	228	53.491	20.558	16.461	1.00 28.53	Α
	MOTA	1292	CA	LYS	Α	228	54.760	20.745	17.149	1.00 32.12	A
	MOTA	1293	CB	LYS	Α	228	54.699	21.974	18.054	1.00 33.81	A
25	ATOM	1294	CG	LYS	Α	228	56.007	22.294	18.765	1.00 41.23	A
	ATOM	1295	CD	LYS	Α	228	57.082	22.725	17.768	1.00 47.57	A
	ATOM	1296	CE	LYS	Α	228	58.401	23.056	18.462	1.00 49.82	A
	ATOM	1297	NZ	LYS	Α	228	59.459	23.425	17.480	1.00 51.49	A
	ATOM	1298	С	LYS	A	228	55.019	19.504	17.985	1.00 33.25	A
30	ATOM	1299	0	LYS	Α	228	54.190	19.129	18.815	1.00 33.70	A
	MOTA	1300	N	VAL	Α	229	56.159	18.860	17.756	1.00 33.64	A
	ATOM	1301	CA	VAL	Α	229	56.516	17.661	18.501	1.00 34.66	A
	MOTA	1302	CB	VAL	Α	229	57.248	16.646	17.609	1.00 33.50	A
	ATOM	1303	CG1	VAL	A	229	57.619	15.419	18.415	1.00 32.34	A
35	ATOM	1304	CG2	VAL	A	229	56.370	16.264	16.436	1.00 34.25	A
	ATOM	1305	C	VAL	Α	229	57.420	18.035	19.668	1.00 37.57	A
	ATOM	1306	0	VAL	A	229	58.581	18.392	19.474	1.00 35.91	A
	ATOM	1307	N	LEU	Α	230	56.877	17.948	20.878	1.00 40.57	Α
	ATOM	1308	CA	LEU	Α	230	57.615	18.289	22.088	1.00 46.10	A
40	ATOM	1309	CB	LEU	Α	230	56.654	18.417	23.270	1.00 44.71	A
	ATOM	1310	CG	LEU	A	230	55.627	19.545	23.207	1.00 44.50	Α
	ATOM	1311	CD1	LEU	Α	230	54.673	19.430	24.383	1.00 44.39	A
	MOTA	1312	CD2	LEU	A	230	56.340	20.885	23.214	1.00 44.81	A
	ATOM	1313	С	LEU	Α	230	58.695	17.279	22.440	1.00 50.42	A
45·	ATOM	1314	0			230	58.603	16.104	22.089	1.00 51.64	A
	ATOM	1315	N			231	59.717	17.756	23.145	1.00 55.81	A
	ATOM	1316	CA	SER	Α	231	60.824	16.914	23.583	1.00 61.14	A
	ATOM	1317	CB			231	62.077	17.200	22.750	1.00 61.27	A
	ATOM	1318	OG			231	62.444	18.568	22.823	1.00 62.85	A.
50	ATOM	1319	C			231	61.124	17.126	25.071	1.00 64.65	A
-	ATOM	1320	0			231	61.392	16.164	25.794	1.00 65.70	A
	ATOM	1321	N			232	61.081	18.387	25.549	1.00 67.54	A
	ATOM	1322	CD			232	60.854	19.651	24.823	1.00 68.60	A
	ATOM	1323	CA			232	61.358	18.655	26.966	1.00 68.74	
55	ATOM	1324	CB			232	61.109	20.158	27.086	1.00 68.83	
	ATOM	1325	CG			232	61.505	20.666	25.737	1.00 68.96	
	ATOM	1326	C			232	60.460	17.846	27.899	1.00 69.17	
	ATOM	1327	ō			232	59.335	17.494	27.541	1.00 69.94	
	ATOM	1328	N			237	57.424	23.198	27.637	1.00 80.06	

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	ATOM	1329	CA	AT.A Z	A 237	56.783	23.047	26.335	1.00 79.29	A
	ATOM	1330	CB		A 237	55.275	22.907	26.512	1.00 78.64	A
	ATOM	1331	C		A 237	57.092	24.239	25.433	1.00 79.07	A
	MOTA	1332	ō		A 237	56.250	25.113	25.249	1.00 79.47	A
5	MOTA	1333	N		A 238	58.297	24.280	24.871	1.00 78.57	A
,	ATOM	1334	CA		A 238	58.683	25.383	23.992	1.00 78.50	A
	ATOM	1335	CB		A 238	60.186	25.347	23.728	1.00 78.50	A
	ATOM	1336	C		A 238	57.920	25.327	22:673	1.00 78.15	´ A
	ATOM	1337	0		A 238	57.243	24.341	22.375	1.00 77.96	Α
10	ATOM	1338	N		A 239	58.027	26.393	21.887	1.00 77.28	A
	ATOM	1339	CA		A 239	57.338	26.452	20.603	1.00 76.27	Α
	ATOM	1340	CB		A 239	55.849	26.489	20.827	1.00 76.61	A
	MOTA	1341	C		A 239	57.766	27.667	19.793	1.00 75.38	A
	ATOM	1342	ō		A 239	58.955	27.955	19.700	1.00 75.89	A
15	ATOM	1343	N		A 240	56.781	28.357	19.214	1.00 73.95	A
13	ATOM	1344	CA		A 240	56.967	29.553	18.389	1.00 71.07	A
	ATOM	1345	CB		A 240	58.151	30.400	18.874	1.00 71.47	A
	ATOM	1346	CG		A 240	59.459	30.055	18.174	1.00 72.06	A
	ATOM	1347		ASN		59.575	30.149	16.943	1.00 72.03	A
20	ATOM	1348		ASN		60.470	29.665	18.964	1.00 71.91	A
	ATOM	1349	C		A 240	57.188	29.178	16.928	1.00 69.41	A
	ATOM	1350	ō		A 240	57.480	28.024	16.624	1.00 70.09	A
	ATOM	1351	Ŋ		A 241	57.055	30.165	16.038	1.00 66.62	A
	ATOM	1352	CA		A 241	57.246	30.013	14.585	1.00 63.94	Α
25	ATOM	1353	C		A 241	55.952	30.080	13.772	1.00 60.63	A
	ATOM	1354	0	ALA .	A 241	55.840	30.880	12.845	1.00 61.29	A
	ATOM	1355	СВ	ALA	A 241	57.979	28.704	14.246	1.00 65.23	A
	ATOM	1356	N	PHE	A 242	54.984	29.236	14.113	1.00 56.72	A
	ATOM	1357	CA	PHE	A 242	53.712	29.196	13.394	1.00 52.53	A
30	ATOM	1358	CB	PHE	A 242	53.419	27.767	12.923	1.00 49.14	A
	ATOM	1359	CG	PHE	A 242	52.040	27.590	12.354	1.00 47.38	A
	ATOM	1360	CD1	PHE	A 242	51.731	28.067	11.085	1.00 47.69	A
	MOTA	1361	CD2	PHE	A 242	51.038	26.975	13.102	1.00 45.45	A
	ATOM	1362			A 242		27.937	10.565	1.00 46.75	A
35	MOTA	1363	CE2		A 242		26.840	12.594	1.00 45.41	A
	MOTA	1364	CZ		A 242		27.323	11.322	1.00 46.55	A
	ATOM	1365	C		A 242		29.688	14.229	1.00 50.08	A
	ATOM	1366	0		A 242		29.505	15.444	1.00 49.86	A
	MOTA	1367	N		A 243		30.305	13.557	1.00 47.67	A A
40	MOTA	1368	CA		A 243		30.809	14.200	1.00 46.21	A
	MOTA	1369	CB		A 243		32.352	14.258	1.00 47.36 1.00 47.54	A
	ATOM	1370			A 243		32.844	14.825 15.109	1.00 47.54	·A
	ATOM	1371			A 243		32.842	13.389	1.00 44.12	A
4.5	ATOM	1372	C		A 243		30.342	12.247	1.00 44.12	A
45	ATOM	1373	0		A 243		29.467	13.985	1.00 40.48	A
	ATOM	1374	N		A 244		28.941	13.306	1.00 37.65	A
	ATOM	1375	CA		A 244 A 244		29.960	12.964	1.00 37.03	. A
	MOTA	1376	C O		A 244		31.168	13.065	1.00 35.92	A
50	MOTA	1377 1378	N		A 244		29.463	12.560	1.00 33.30	A
50	ATOM	1379	CA		A 245		30.312	12.184	1.00 30.20	A
	ATOM ATOM	1380	CB		A 245		29.450	11.829	1.00 32.00	A
	ATOM	1381			A 245		28.573	10.755	1.00 32.81	A
	ATOM	1382			A 245		30.319	11.390	1.00 28.34	A
55	ATOM	1383	C		A 245		31.296	13.296	1.00 27.96	A
55	ATOM	1384	ō		A 245		30.907	14.434	1.00 25.46	A
	ATOM	1385	N		A 246		32.576	12.938	1.00 25.22	A
	ATOM	1386	CA		A 246		33.675	13.867	1.00 23.27	A
	MOTA	1387	CB		A 246		34.955	13.082	1.00 22.94	A

	ATOM	1388	C	ALA	Α	246		42.178	33.475	14.934	1.00 21.27	A
	MOTA	1389	0	ALA	Α	246		42.431	33.705	16.114	1.00 20.93	A
	MOTA	1390	N	GLN	A	247		40.988	33.047	14.536	1.00 19.67	A
	ATOM	1391	CA	GLN	Α	247		39.911	32.886	15.504	1.00 20.17	A
5	ATOM	1392	CB	GLN	A`	247		38.608	32.535	14.779	1.00 21.89	A
	ATOM	1393	CG	GLN	Α	247		38.522	33.076	13.355	1.00 26.18	A
	ATOM	1394	CD	GLN	Α	247		37.220	33.794	13.064	1.00 27.30	A
	ATOM	1395	OE1	GLN	Α	247		36.172	33.447	13.605	1.00 30.13	A
	ATOM	1396	NE2	GLN	Α	247		37.278	34.792	12.189	1.00 28.70	A
10	ATOM	1397	С	GLN	Α	247		40.181	31.849	16.595	1.00 19.43	A
	ATOM	1398	0	GLN	Α	247		39.546	31.883	17.648	1.00 18.93	A
	MOTA	1399	N	TYR				41.132	30.948	16.359	1.00 18.60	A
	ATOM	1400	CA	TYR				41.441	29.896	17.329	1.00 19.20	A
	ATOM	1401	CB	TYR				41.333	28.529	16.642	1.00 17.53	A
15	ATOM	1402	CG	TYR				40.013	28.362	15.927	1.00 19.32	A
	ATOM	1403		TYR				38.859	28.010	16.625	1.00 17.69	Α
	ATOM	1404		TYR			•	37.617	27.976	15.990	1.00 18.18	A
	ATOM	1405		TYR				39.897	28.664	14.569	1.00 16.87	A
	ATOM	1406		TYR				38.665	28.635	13.924	1.00 19.17	A
20	ATOM	1407	CZ			248		37.527	28.295	14.643	1.00 19.46	A
	ATOM	1408	OH			248		36.299	28.311	14.023	1.00 18.98	Α
	ATOM	1409	C			248		42.810	30.039	17.993	1.00 20.42	A
	ATOM	1410	ō	,		248		43.208	29.191	18.792	1.00 19.19	A
	ATOM	1411	N			249		43.523	31.114	17.673	1.00 20.20	A
25	ATOM	1412	CA			249		44.841	31.343	18.251	1.00 20.91	A
	ATOM	1413	CB			249		45.542	32.532	17.570	1.00 21.18	A
	ATOM	1414		VAL				46.821	32.896	18.317	1.00 22.45	A
	ATOM	1415		VAL				45.862	32.170	16.139	1.00 24.01	A
	ATOM	1416	C			249		44.764	31.606	19.750	1.00 21.52	A
30	ATOM	1417	0			249		43.915	32.368	20.216	1.00 22.72	~ A
	ATOM	1418	N			250		45.654	30.965	20.503	1.00 20.70	A
	ATOM	1419	CA			250		45.697	31.133	21.951	1.00 21.65	A
	ATOM	1420	СВ			250		46.370	29.919	22.613	1.00 22.02	A
	ATOM	1421	OG	SER	Α	250		47.692	29.725	22.132	1.00 22.12	A
35	ATOM	1422	C	SER	Α	250		46.476	32.402	22.280	1.00 22.13	A
	ATOM	1423	0			250		47.332	32.828	21.511	1.00 22.77	A
	ATOM	1424	N	PRO	Α	251		46.180	33.029	23.425	1.00 22.23	A
	ATOM	1425	CD	PRO	Α	251		45.163	32.684	24.433	1.00 22.97	A
	ATOM	1426	CA	PRO	Α	251		46.893	34.254	23.800	1.00 22.52	A
40	ATOM	1427	СВ	PRO	Α	251		46.233	34.650	25.127	1.00 23.06	A
	ATOM	1428	CG	PRO	Α	251		45.726	33.329	25.676	1.00 22.55	A
	ATOM	1429	C	PRO	Α	251		48.414	34.115	23.907	1.00 22.15	À
	ATOM	1430	0	PRO	Α	251		49.143	35.047	23.563	1,00 22.62	A
	ATOM	1431	^ N	GLU	Α	252		48.901	32.966	24.367	1.00 20.69	A
45	ATOM	1432	CA	GLU	Α	252		50.347	32.772	24.500	1.00 21.40	A
	ATOM	1433	CB			252		50.673	31.382	25.071	1.00 20.59	A
	ATOM	1434	CG	GLU	Α	252		49.993	30.232	24.352	1.00 21.91	A
•	ATOM	1435	CD			252		48.691	29.822	25.014	1.00 21.51	A
	ATOM	1436		GLU				47.989	30.707	25.550	1.00 21.46	A
50	MOTA	1437		GLU				48.367	28.613	24.993	1.00 20.23	A
	ATOM	1438	С			252		51.071	32.970	23.167	1.00 22.99	Α
	ATOM	1439	0	GLU	Α	252		52.191	33.480	23.136	1.00 23.17	A
	ATOM	1440	N			253		50.441	32.576	22.064	1.00 23.00	A
	ATOM	1441	CA			253		51.068	32.753	20.758	1.00 25.62	A
55	MOTA	1442	CB			253		50.277	32.029	19.669	1.00 26.75	A
	ATOM	1443	CG	LEU	A	253		50.743	30.620	19.296	1.00 31.87	A
	MOTA	1444	CD1	LEU	A	253		50.433	29.651	20.422	1.00 31.81	Α
	MOTA	1445	CD2	LEU	A	253		50.044	30.179	18.015	1.00 31.86	A
	ATOM	1446	С	LEU	A	253		51.201	34.228	20.371	.1.00 26.94	A

ATOM 1484 OG SER A 258 54.741 30.892 24.734 1.00 54 ATOM 1485 C SER A 258 53.735 29.415 22.342 1.00 64 ATOM 1486 O SER A 258 52.617 29.932 22.417 1.00 64 ATOM 1487 N ALA A 259 53.917 28.105 22.204 1.00 64 ATOM 1488 CA ALA A 259 52.793 27.180 22.127 1.00 65 ATOM 1489 CB ALA A 259 52.551 26.779 20.684 1.00 65 ATOM 1490 C ALA A 259 52.551 26.779 20.684 1.00 65 ATOM 1491 O ALA A 259 53.042 25.940 22.977 1.00 65 ATOM 1492 N CYS A 260 51.975 25.428 23.579 1.00 65 ATOM 1493 CA CYS A 260 51.975 25.428 23.579 1.00 65 ATOM 1494 CB CYS A 260 52.056 24.244 24.425 1.00 65 ATOM 1495 SG CYS A 260 50.846 25.739 26.469 1.00 65 ATOM 1496 C CYS A 260 50.846 25.739 26.469 1.00 65 ATOM 1497 O CYS A 260 50.786 23.435 24.224 1.00 65 ATOM 1498 N LYS A 261 50.706 22.277 24.868 1.00 65 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 65 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 65 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 65 ATOM 1500 CB LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 65 ATO		
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S ATOM 1451 CG LEU A 254		·A
ATOM 1452 CD1 LEU A 254 46.459 36.724 19.932 1.00 2 ATOM 1453 CD2 LEU A 254 48.236 36.597 18.177 1.00 3 ATOM 1455 C LEU A 254 51.134 37.314 21.537 1.00 3 ATOM 1455 N THR A 255 51.292 36.821 22.758 1.00 3 ATOM 1456 N THR A 255 51.292 36.821 22.758 1.00 3 ATOM 1457 CA THR A 255 51.292 36.821 22.758 1.00 3 ATOM 1459 OG1 THR A 255 51.368 37.478 25.127 1.00 3 ATOM 1459 OG1 THR A 255 51.368 37.478 25.127 1.00 3 ATOM 1450 CG2 THR A 255 51.368 37.478 25.127 1.00 3 ATOM 1460 CG2 THR A 255 51.188 36.106 25.494 1.00 3 ATOM 1461 C THR A 255 51.188 36.106 25.494 1.00 3 ATOM 1461 C THR A 255 53.477 37.035 23.910 1.00 4 ATOM 1462 O THR A 255 53.477 37.035 23.910 1.00 4 ATOM 1463 N GLU A 256 53.617 35.747 24.189 1.00 4 ATOM 1464 CA GLU A 256 54.932 35.144 24.382 1.00 4 ATOM 1465 CB GLU A 256 54.932 35.144 24.382 1.00 4 ATOM 1466 CG GLU A 256 54.514 34.786 26.862 1.00 5 ATOM 1466 CG GLU A 256 54.514 34.786 26.862 1.00 5 ATOM 1468 OE1 GLU A 256 54.563 33.780 27.893 1.00 5 ATOM 1469 OE2 GLU A 256 54.563 33.780 27.893 1.00 6 ATOM 1470 C GLU A 256 54.766 32.776 28.107 1.00 6 ATOM 1470 C GLU A 256 55.475 34.456 23.137 1.00 6 ATOM 1470 LA 256 55.656 33.996 28.494 1.00 6 ATOM 1470 C GLU A 256 56.516 33.995 23.127 1.00 6 ATOM 1470 C GLU A 256 56.516 33.995 23.127 1.00 5 ATOM 1471 CB LYS A 257 55.064 33.780 27.893 1.00 5 ATOM 1470 C GLY A 256 56.516 33.995 23.127 1.00 5 ATOM 1471 CB LYS A 257 55.064 33.780 27.993 1.00 5 ATOM 1470 CB LYS A 257 55.064 33.794 20.227 1.00 5 ATOM 1470 CB LYS A 257 55.064 33.794 22.227 1.00 5 ATOM 1470 CB LYS A 257 55.064 33.794 22.227 1.00 5 ATOM 1478 NZ LYS A 257 55.064 33.794 22.227 1.00 5 ATOM 1478 NZ LYS A 257 55.064 33.795 22.127 1.00 5 ATOM 1480 CB LYS A 257 55.064 33.795 22.127 1.00 5 ATOM 1480 CB LYS A 257 56.244 34.25 20.277 1.00 5 ATOM 1480 CB LYS A 257 56.244 34.502 20.277 1.00 5 ATOM 1480 CB LYS A 257 56.244 34.25 20.277 1.00 5 ATOM 1480 CB LYS A 257 56.246 32.302 21.138 1.00 5 ATOM 1480 CB LYS A 257 56.246 32.302 21.138 1.00 5 ATOM 1480 CB LYS A 257 56.246 32.302 22.477 1.00 6 ATOM 1480 CB LYS A		A
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45 ATOM 1491 O ALA A 259 54.172 25.459 23.086 1.00 2 ATOM 1492 N CYS A 260 51.975 25.428 23.579 1.00 2 ATOM 1493 CA CYS A 260 52.056 24.244 24.425 1.00 2 ATOM 1494 CB CYS A 260 52.056 24.244 24.425 1.00 2 ATOM 1495 SG CYS A 260 52.183 24.654 25.892 1.00 2 ATOM 1496 C CYS A 260 50.846 25.739 26.469 1.00 2 ATOM 1497 O CYS A 260 50.786 23.435 24.224 1.00 2 ATOM 1498 N LYS A 261 49.892 23.856 23.495 1.00 2 ATOM 1498 N LYS A 261 50.706 22.277 24.868 1.00 2 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 2 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 2 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 2 ATOM 1501	34.16	A
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ATOM 1495 SG CYS A 260 50.846 25.739 26.469 1.00 3 50 ATOM 1496 C CYS A 260 50.786 23.435 24.224 1.00 3 ATOM 1497 O CYS A 260 49.892 23.856 23.495 1.00 3 ATOM 1498 N LYS A 261 50.706 22.277 24.868 1.00 3 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 3 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 3 55 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 3		A A
50 ATOM 1496 C CYS A 260 50.786 23.435 24.224 1.00 2 ATOM 1497 O CYS A 260 49.892 23.856 23.495 1.00 2 ATOM 1498 N LYS A 261 50.706 22.277 24.868 1.00 2 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 2 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 2 55 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 2		A
ATOM 1497 O CYS A 260 49.892 23.856 23.495 1.00 2 ATOM 1498 N LYS A 261 50.706 22.277 24.868 1.00 2 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 2 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 2 55 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 2		A.
ATOM 1498 N LYS A 261 50.706 22.277 24.868 1.00 2 ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 2 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 3 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 3		A
ATOM 1499 CA LYS A 261 49.526 21.434 24.744 1.00 2 ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 2 55 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 2		A
ATOM 1500 CB LYS A 261 49.619 20.243 25.696 1.00 3 55 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00 3		A
55 ATOM 1501 CG LYS A 261 50.716 19.253 25.347 1.00	23.28	A
)) A10:: 2502 CG 210 :: 202	27.44	Α
ATOM 1502 CD LYS A 261 50.732 18.117 26.350 1.00	29.98	A
	32.34	A
ATOM 1504 NZ LYS A 261 51.940 16.121 27.153 1.00	33.28	A
ATOM 1505 C LYS A 261 48.268 22.229 25.062 1.00	19.20	A

	MOTA	1506	0	LYS	A	261	47.253	22.092	24.387	1.00 18.	08 A
	ATOM	1507	И	SER	A	262	48.358	23.068	26.089	1.00 16.	92 A
	ATOM	1508	CA	SER	A	262	47.235	23.883	26.534	1.00 18.	13 A
	ATOM	1509	CB	SER	A	262	47.644	24.698	27.770	1.00 18.	27 A
5	ATOM	1510	OG	SER	Α	262	46.517	25.258	28.421	1.00 22.	53 A
	MOTA	1511	C	SER	A	262	46.736	24.811	25.424	1.00 16.	77 A
	ATOM	1512	0	SER	A	262	45.591	25.254	25.450	1.00 15.	69 A
	ATOM	1513	N	SER	Α	263	47.595	25.118	24.456	1.00 16.	44 A
	. ATOM	1514	CA	SER	Α	263	47.175	25.970	23.347	1.00 16.	89 A
10	ATOM	1515	CB	SER	Α	263	48.340	26.228	22.382	1.00 18.	49 A
	ATOM	1516	OG	SER	Α	263	49.402	26.909	23.031	1.00 22.	10 A
	ATOM	1517	C	SER	A	263	46.040	25.257	22.612	1.00 17.	79 A
	ATOM	1518	0	SER	A	263	45.099	25.898	22.148	1.00 17.	57 A
	ATOM	1519	N	ASP	Α	264	46.119	23.928	22.517	1.00 16.	30 A
15 .	ATOM	1520	CA	ASP	A	264	45.069	23.166	21.836	1.00 16.	72 A
	MOTA	1521	CB	ASP	A	264	45.483	21.704	21.620	1.00 15.	92 A
	MOTA	1522	CG	ASP	Α	264	46.544	21.539	20.548	1.00 17.	93 A
	ATOM	1523	OD1	ASP	Α	264	46.642	22.412	19.661	1.00 16.	78 A
	MOTA	1524	OD2	ASP	Α	264	47.265	20.515	20.579	1.00 16.	64 A
20 -	MOTA	1525	С	ASP	Α	264	43.773	23.194	22.646	1.00 17.	67 A
	MOTA	1526	0	ASP	Α	264	42.681	23.197	22.076	1.00 18.	27 A
	MOTA	1527	N	LEU	Ά	265	43.898	23.205	23.974	1.00 15.	49 A
	MOTA	1528	CA	LEU	Α	265	42.730	23.232	24.849	1.00 14.	.75 A
	MOTA	1529	CB	LEU	Α	265	43.147	23.038	26.313	1.00 11.	.38 A
25	ATOM	1530	CG	LEU	Α	265	43.711	21.641	26.621	1.00 14.	04 A
	ATOM	1531	CD1	LEU	Α	265	44.249	21.579	28.052	1.00 13.	96 A
	MOTA	1532	CD2	LEU	Α	265	42.619	20.603	26.416	1.00 11.	62 A
	MOTA	1533	С	LEU	Α	265	41.999	24.557	24.675	1.00 15.	13 A
	MOTA	1534	0	LEU	A	265	40.777	24.620	24.785	1.00 16.	.75 A
30	ATOM	1535	N	TRP	Α	266	42.746	25.622	24.405	1.00 16.	.08 A
	ATOM	1536	CA	TRP	A	266	42.118	26.918	24.184	1.00 16.	96 A
	ATOM	1537	CB			266	43.176	28.015	24.023	1.00 17.	28 A
	ATOM	1538	CG	TRP	Α	266	42.618	29.326	23.521	1.00 20.	54 A
	ATOM	1539		TRP			42.313	30.490	24.301	1.00 20.	.07 A
35	ATOM	1540		TRP			41.782	31.459	23.417	1.00 20.	46 A
	ATOM	1541		TRP			42.435	30.810	25.660	1.00 20.	.68 A
	ATOM	1542		TRP			42.270	29.631	22.231	1.00 19	.53 A
	MOTA	1543		TRP			41.769	30.908		1.00 19	61 A
	MOTA	1544		TRP			41.372	32.727	23.850	1.00 20	.90 A
40 -	ATOM	1545	CZ3	TRP	Α	266	42.026	32.073	26.091	1.00 19	.45 A
	MOTA	1546		TRP			41.501	33.015	25.185	1.00 20.	71 A
	MOTA	1547	С			266	41.284	26.795	22.913	1.00 17	. 22 A
	MOTA	1548	0	TRP	Α	266	40.139	27.240	22.863	1.00 18	.03 A
	ATOM	1549	N	ALA			41.863	26.181	21.886	1.00 17	.50 A
45	MOTA	1550	CA	ALA	А	267	41.155	25.990	20.626	1.00 16.	.16 A
	MOTA	1551	CB	ALA			42.050	25.290	19.621	1.00 14	
	MOTA	1552	С			267	39.901	25.159	20.891	1.00 16	.28 A
	MOTA	1553	0	ALA			38.835	25.436	20.346	1.00 16	.46 A
	ATOM	1554	N	LEU			40.031	24.144	21.739	1.00 16	.57 A
50	ATOM	1555	CA	LEU			38.890	23.299	22.084	1.00 17	
	ATOM	1556	CB			268	39.292	22.260	23.139	1.00 15	
	ATOM	1557	CG	LEU			38.158	21.429	23.754	1.00 19	
	ATOM	1558		LEU			3.7.505	20.578	22.678	1.00 16	
	ATOM	1559		LEU			38.718	20.537	24.881	1.00 17	
55	ATOM	1560	C			268	37.766	24.179	22.628	1.00 15	
	ATOM	1561	ō			268	36.603	24.031	22.247	1.00 15	
	ATOM	1562	N			269	38.119	25.099	23.520	1.00 14	
	ATOM	1563	CA			269	37.124	25.989	24.092	1.00 13	
	ATOM	1564	C			269	36.406	26.808	23.031	1.00 14	
						-					

	MOTA	1565	0	GLY	A	269		35.193	27.014	23.114	1.00	14.76	A
	MOTA	1566	N	CYS	Α	270		37.146	27.279	22.030	1.00	13.86	A
	ATOM	1567	CA	CYS	Α	270		36.539	28.061	20.958	1.00	16.80	A
	ATOM	1568	CB	CYS	A	270		37.611	28.634	20.023	1.00	15.97	A
5	ATOM	1569	SG	CYS	Ą	270		38.751	29.810	20.780	1.00	20.48	A
	ATOM	1570	С	CYS	Α	270		35.598	27.175	20.140	1.00	17.50	A
	ATOM	1571	0	CYS	Α	270		34.516	27.604	19.741	1.00	18.38	A
	ATOM	1572	N	ILE	A	271		36.022	25.939	19.887	1.00	16.99	A
	ATOM	1573	CA	ILE				35.221	25.004	19.104	1.00	16.66	A
10	ATOM	1574	CB	ILE				36.038	23.741	18.778	1.00	16.53	A
	ATOM	1575		ILE				35.155	22.694	18.102	1.00	16.34	A
	ATOM	1576		ILE				37.222	24.129	17.882	1.00	15.59	Α
	ATOM	1577		ILE				38.239	23.018	17.690		14.88	A
	ATOM	1578	C	ILE				33.920	24.626	19.809	1.00	16.74	A
15	ATOM	1579	Ö	ILE				32.865	24.576	19.179		17.12	A
10	ATOM	1580	N	ILE				33.990	24.357	21.111		16.13	A
	ATOM	1581	CA	ILE				32.785	24.021	21.862		18.30	A
	ATOM	1582	CB	ILE				33.097	23.747	23.346		17.77	A
	ATOM	1583		ILE				31.796	23.666	24.152		17.96	A
20	ATOM	1584		ILE				33.877	22.437	23.481		19.55	A
20	MOTA	1585		ILE				34.446	22.217	24.886		18.64	A
	ATOM	1586	C	ILE				31.824	25.207	21.776		19.51	A
	ATOM	1587	o	ILE			•	30.624	25.037	21.554		20.44	A
	ATOM	1588	N	TYR				32.362	26.409	21.947		18.52	A
25	ATOM	1589	CA			273		31.553	27.615	21.881		20.48	A
23	ATOM	1590	CB			273		32.418	28.847	22.162		18.98	A
	ATOM	1591	CG	TYR				31.663	30.161	22.125		20.26	A
	ATOM	1592		TYR				31.229	30.709	20.916		20.67	A
	ATOM	1593		TYR				30.536	31.917	20.880	1.00	20.98	A
30	ATOM	1594	CD2					31.383	30.857	23.302		19.82	A
-	ATOM	1595	CE2					30.691	32.062	23.280		20.62	A
	ATOM	1596	CZ			273		30.271	32.587	22.067	1.00	21.15	A
	ATOM	1597	OH	TYR				29.588	33.776	22.049	1.00	21.86	A
	ATOM	1598	C			273		30.902	27.730	20.507		21.54	A
35	ATOM	1599	ō	TYR				29.719	28.049	20.401	1.00	22.80	A
	ATOM	1600	N			274		31.676	27.454	19.461	1.00	21.05	A
	ATOM	1601	CA			274		31.176	27.538	18.095	1.00	21.48	A
	ATOM	1602	CB			274		32.323	27.341	17.097	1.00	21.41	Α
	MOTA	1603	CG	GLN	Α	274		31.934	27.596	15.645	1.00	23.15	Α
40	MOTA	1604	CD	GLN	Α	274		33.131	27.588	14.706	1.00	24.80	Α
	ATOM	1605	OE1	GLN				34.276	27.446	15.139	1.00	22.51	Α
	ATOM	160 ⁶	NE2	GLN	A	274		32.870	27.750	13.413	1.00	22.96	Α
	MOTA	1607	C	GLN	Α	274		30.076	26.517	17.828	1.00	21.51	A
	MOTA	1608	0	GLN	Α	274		29.123	26.806	17.108	1.00	20.50	A
45	MOTA	1609	N	LEU	Α	275		30.207	25.324	18.403	1.00	21.44	A
	ATOM	1610	CA	LEU				29.196	24.282	18.208	1.00	20.95	· A
	ATOM	1611	CB			275		29.645	22.958	18.846	1.00	19.11	A
	ATOM	1612	CG	LEU	Α	275		30.775	22.182	18.159	1.00	21.43	A
	MOTA	1613	CD1	LEU				31.118	20.936	18.963	1.00	17.64	A
50	ATOM	1614	CD2	LEU	Α	275		30.342	21.795	16.754		20.34	A
	MOTA	1615	С	LEU	Α	275		27.860	24.697	18.815	1.00	21.32	A
	MOTA	1616	Ο,	LEU.	Α	275		26.802	24.461	18.229	1.00	19.75	A
	ATOM	1617	N	VAL	A	276		27.921	25.322	19.987		19.10	A
	MOTA	1618	CA	VAL	Α	276		26.724	25.750	20.702		22.47	A
55	ATOM	1619	CB	VAL	Α	276		27.011	25.882	22.217		20.87	A
	ATOM	1620	CG1	VAL	A	276		25.742	26.291	22.957		19.68	A
	ATOM	1621	CG2	VAL	A	276		27.550	24.558	22.766		19.43	Α
	MOTA	1622	, C	VAL	Α	276		26.127	27.075	20.211		23.89	A
	MOTA	1623	o	VAL	Α	276		24.910	27.199	20.070	1.00	24.90	A

	ATOM	1624	N	ALA	Α	277		26.	983	28.062	19.965	1.00	24.56	A
	ATOM	1625	CA	ALA	A	277		26.	533	29.374	19.518	1.00	24.72	A
	ATOM	1626	CB	ALA	A	277		27.	504	30.444	19.999	1.00	24.36	A
	ATOM	1627	C	ALA	A	277		26.	378	29.458	18.005	1.00	25.76	A
5	ATOM	1628	0	ALA	A	277		25.	577	30.242	17.502	1.00	26.39	A
	MOTA	1629	N	GLY	A	278		27.	142	28.651	17.280		25.13	A
	MOTA	1630	CA	GLY	A	278		27.	062	28.673	15.834		25.58	A
	ATOM	1631	С	GLY	Α	278	•	28.	163	29.524	15.231		26.50	A
	ATOM	1632	0	GLY	Α	278		28.	374	29.510	14.015		28.17	A
10	MOTA	1633	N	LEU	Α	279		28.	866	30.262	16.086	1.00	24.44	A
	ATOM	1634	CA	LEU	Α	279		29.	962	31.130	15.656		25.21	A
	MOTA	1635	CB	LEU	Α	279		29.	468	32.575	15.500		25.78	A
	MOTA	1636	CG	LEU	Α	279		28.	364	32.899	14.490		28.17	A
	MOTA	1637	CD1	LEU	Α	279		27.	922	34.344	14.684	1.00	26.60	A
15	MOTA	1638	CD2	LEU	A	279		28	862	32.670	13.071	1.00	26.52	A
	MOTA	1639	С	LEU	A	279		31	. 093	31.116	16.687	1.00	23.47	A
	MOTA	1640	0	LEU	A	279		30	848	30.994	17.882	1.00	24.44	A
	MOTA	1641	N	PRO	Α	280		32	.349	31.239	16.236	1.00	23.35	A
	MOTA	1642	CD	PRO	Α	280		32	.831	31.404	14.855	1.00	22.26	A
20	MOTA	1643	CA	PRO	A	280		33	.464	31.239	17.189	1.00	23.81	A
	ATOM	1644	CB.	PRO	Α	280		34	. 692	31.293	16.282	1.00	23.24	· A
	ATOM	1645	CG	PRO	A	280		34	.189	32.020	15.073		24.89	A
	MOTA	1646	C	PRO	Α	280		33	.353	32.444	18.137		22.69	A
	ATOM	1647	0	PRO	A	280		32	.750	33.457	17.788		22.11	A
25	MOTA	1648	N	PRO	Α	281		33	. 939	32.344	19.345		23.06	, A
	MOTA	1649	CD	PRO	A	281		34	.810	31.223	19734		21.37	A
-	MOTA	1650	CA	PRO	A	281		33	. 935	33.375	20.395		23.67	A
	MOTA	1651	CB	PRO	A	281		34	.781	32.751	21.509		24.89	A
	MOTA	1652	CG	PRO	Α	281		34	.749	31.287	21.219		25.24	Α
30	MOTA	1653	C	PRO	А	281		34	.481	34.752	20.017		23.75	A
	MOTA	1654	0	PRO	A	281		33	.869	35.781	20.317		21.02	A
	ATOM	1655	N	PHE	А	282		35	.644	34.763	19.379		22.17	A
	MOTA	1656	CA	PHE	A.	282		36	.293	36.007	18.998		23.16	A
	MOTA	1657	CB	PHE	A	282		37	.765	35.943	19.406		21.01	A
35	MOTA	1658	CG	PHE	A	282			. 975	35.482	20.822		22.66	A
	ATOM	1659	CD1	PHE	Α	282			.806	36.361	21.888		20.06	A
	ATOM	1660	CD2	PHE	A	282		38	.291	34.151	21.093		20.72	A
	ATOM	1661	CE1	PHE	Α	282		37	.947	35.921	23.206		22.66	A.
	ATOM	1662	CE2	PHE	A	282			.433	33.702	22.405		20.97	. A
40	ATOM	1663	CZ	PHE	Α	282			.261	34.590	23.466		19.58	A
	ATOM	1664	C			282			.169	36.263	17.503		24.39	A
	ATOM	1665	0			282			.802	35.585	16.694		25.80	A -
	.ATOM	1666	N			283			.355	37.248	17.142		24.99	A
	MOTA	1667	CA			283			.141	37.594	15.741		26.33	A
45	MOTA	1668	CB			283			.721	37.209	15.316		28.91	A
	MOTA	1669	CG			283			.293	35.808	15.724		30.27	A
	MOTA	1670	CD			283			.904	35.493	15.188		33.36	A
	MOTA	1671	NE			283			.890	36.392	15.733		32.76	A
	MOTA	1672	\mathbf{cz}			283			.372	36.287	16.952		34.79	A
50	MOTA	1673		ARG					.767	35.317	17.768		35.77	A
	MOTA	1674	NH2	ARG					.458	37.156	17.359		36.12	A
	MOTA	1675	C			283			.328	39.096	15.544		26.47	A
	ATOM	1676	0			283			.029	39.888	16.438		26.28	A
	ATOM	1677				284			.818	39.486	14.373		26.70	A A
55	ATOM	1678	CA			284			.033	40.899	14.079		27.84	A A
	MOTA	1679	CB			284			.188	41.442	14.914			
	ATOM	1680	C			284			.327	41.077	12.602		28.35	A A
	ATOM	1681	0			284			.560	40.101	11.891			A A
	MOTA	1682	N	GLY	A	285		36	.332	42.329	12.153	1.00	29.29	A

	MOTA	1683	CA	GLY	A	285		36	.577	42.63	31	10.753		29.52		A
	MOTA	1684	C	GLY	A	285		37	.893	42.15	56	10.168		30.12		A
	MOTA	1685	0	GLY	A	285		37	.974	41.86	62	8.976	1.00	30.60		A
	MOTA	1686	N	ASN	Α	286		38	.939	42.09	97	10.983		28.49		A
5	MOTA	1687	CA	ASN	Α	286		40	.231	41.64	44	10.489		26.71		A
	ATOM	1688	CB	ASN	Α	286		41	.050	42.82	25	9.945		26.11		A
	MOTA	1689	CG	ASN	A	286		41	.310	43.90	00	10.990		27.83		A
	ATOM	1690	OD1	ASN	Α	286		41	.877	43.63	31	12.049		27.84		Α
	MOTA	1691	ND2	ASN	Α	286		40	.908	45.13	31	10.685		25.95		A
10	ATOM .	1692	С	ASN	Α	286		40	.997	40.92	24	11.584		26.03		A
	ATOM	1693	0	ASN	Α	286		40	.540	40.8	51	12.723		25.66		Α
	ATOM	1694	N	GLU	Α	287		42	.162	40.3	91	11.239		24.81		Α
	ATOM	1695	CA	GLU	Α	287		42	.965	39.6	62	12.206		27.59		Α
	MOTA	1696	CB	GLU	Α	287		44	.145	38.9	85	11.510		30.17		Α
15	ATOM	1697	CG	GLU	Α	287		43.	.776	37.6	32	10.931		38.21		A
	MOTA	1698	CD	GLU	Α	287		44	.900	36.9		10.140		41.86		A
	MOTA	1699		GLU					.061	37.0		10.608		43.08		A
	MOTA	1700	OE2						.612	36.4		9.052		45.22		A
	ATOM	1701	C			287			.459	40.4		13.383		25.05		A
20	MOTA	1702	0			287			.382	40.0		14.521		26.41		A
	MOTA	1703	N			288			.966	41.6		13.122		23.04		A.
	MOTA	1704	CA			288			.460	42.5		14.205		22.34		A
	ATOM	1705	CB			288			.867	43.9		13.691		21.07		A
	MOTA	1706	CG			288			.275	44.8		14.805		0 21.07 0 21.23		A A
25	ATOM	1707		TYR					.533	44.7		15 405		0 20.43	į	A
	MOTA	1708	CEI						.891	45.5		16.475 15.302		0 22.32		A
	MOTA	1709	CD2			288			.380 .725	45.8 46.6		16.373		0 23.28		A
	ATOM	1710	CE2			288 288	-		.981	46.5		16.953		0 22.96		A
20	ATOM	1711	CZ OH			288			.316	47.3		18.024		0 23.18		A
30	ATOM	1712 1713	C			288			.402	42.6		15.288		0 21.38		A
	ATOM ATOM	1713	0			288			.710	42.6		16.473		0 22.09		Α
	ATOM	1715	N			289			.159	42.9		14.874		0 21.88		Α
	ATOM	1716	CA			289			.055	43.1		15.811		0 21.98		Α
35	ATOM	1717	CB			289			.821	43.6		15.078		0 22.90		Α
55	ATOM	1718	CG			289			.896	45.1		14.601	1.0	0 26.52		Α
	ATOM	1719		LEU					.706	45.4	36	13.696	1.0	0 26.55		Α
	MOTA	1720		LEU					.914	46.0	71	15.807	1.0	0 23.13		Α
	ATOM	1721	C	LEU	Α	289		40	.686	41.8	49	16.560	1.0	0 21.24		Α
40	MOTA	1722	0	LEU	Α	289		40	.256	41.8	97	17.715	1.0	0 20.72		Α
	ATOM	1723	N	ILE	Α	290		40	.843	40.7	80	15.900	1.0	0 19.62		A
	MOTA	1724	CA	ILE	A	290		40	.538	39.4	33	16.533	1.0	0 18.54		Α
	MOTA	1725	CB	ILE	Α	290		40	.560	38.2	81	15.509	. 1.0	0 18.52		À
	MOTA	1726	CG2	ILE	Α	290			.503	36.9	34	16.234		0 17.63		A
45	ATOM	1727		ILE					.378	38.4		14.545		0 18.88		A
	ATOM	1728	CD1	ILE					.421	37.4		13.357		0 19.81		A
	MOTA	1729	С			290			578	39.1		17.618		0 19.09		A
	MOTA	1730	0			290			236	38.7		18.737		0 18.20		A
	ATOM	1731	N			291			.849	39.3		17.286		0 18.76		A
50	MOTA	1732	CA			291			.925	39.1		18.247		0 20.75		A
	MOTA	1733	CB			291			.286	39.4		17.606		0 20.71		A
	ATOM	1734	CG			291			.644	38.4		16.503		0 22.92 0 22.98		A A
	ATOM	1735		PHE					.065	37.2		16.443		0 22.98		A
	ATOM	1736		PHE					.588	38.8		15.543 15.440		0 22.91		A
55	MOTA	1737		PHE					.423	36.3 37.9		14.535		0 24.51		A
•	MOTA	1738	CEZ			291			5.954 5.370	36.6		14.535		0 23.29		A
	ATOM	1739	C			291			3.739	40.0		19.451		0 23.23		A
	MOTA	1740 1741	0			291			3.992	39.6		20.593		0 22.32		A
	MOTA	1/41	J			1,		4.				20.000				

	MOTA	1742	N	GLN	A	292	43.284	41.275	19.178	1.00 23.27	A
	MOTA	1743	CA	GLN	А	292	43.055	42.264	20.216	1.00 24.01	A
	MOTA	1744	CB	GLN	A	292	42.574	43.559	19.562	1.00 25.77	A
	MOTA	1745	CG	GLN	A	292	42.577	44.773	20.447	1.00 28.45	A
5	MOTA	1746	CD	GLN	Α	292	42.469	46.057	19.638	1.00 29.83	A
	ATOM	1747	OE1	GLN	Α	292	41.520	46.244	18.872	1.00 27.16	A
	ATOM	1748	NE2	GLN	Α	292	43.449	46.944	19.799	1.00 27.61	
	ATOM	1749	С	GLN	Α	292	42.018	41.733	21.204	1.00 22.97	A
	MOTA	1750	0 -	GIM	Α	292	42.200	41.832	22.415	1.00 21.64	
10	MOTA	1751	N	LYS			40.937	41.154	20.687	1.00 21.82	
•	MOTA	1752	CA	LYS			39.895	40.612	21.558	1.00 22.18	
	MOTA	1753	CB	LYS			38.664	40.223	20.740	1.00 22.69	
	MOTA	1754	CG	LYS			37.919	41.407	20.153	1.00 25.78	
	MOTA	1755	CD	LYS			36.651	40.961	19.429	1.00 27.88	
15	ATOM	1756	CE			293	35.857	42.161	18.926	1.00 30.85	
	MOTA	1757	NZ			293	34.612	41.750	18.214	1.00 32.98	
	MOTA	1758	С			293	40.398	39.398	22.343	1.00 21.20	
	MOTA	1759	0			293	40.041	39.204	23.509	1.00 22.01	
	ATOM	1760	N			294	41.226	38.583	21.702	1.00 19.91	
20	MOTA	1761	CA			294	41.774	37.394	22.347	1.00 20.28	
	MOTA	1762	CB			294	42.631	36.575	21.349	1.00 18.98	_
	MOTA	1763	CG2			294	43.481	35.550	22.098	1.00 17.70	
	ATOM	1764		ILE			41.716	35.897	20.318	1.00 17.93	
-	MOTA	1765	CD1			294	42.467	35.237	19.178	1.00 16.21	
25	MOTA	1766	C			294	42.618	37.727	23.587	1.00 21.94	
	ATOM	1767	0			294	42.366	37.199	24.673	1.00 20.86	
	ATOM	1768	N			295	43.610	38.600	23.439	1.00 21.88	
	ATOM	1769	CA			295	44.461	38.934	24.582	1.00 24.25	
	MOTA	1770	CB			295	45.668	39.805	24.175	1.00 23.93	
30	MOTA	1771		ILE			46.514	39.066	23.140	1.00 24.61	
	ATOM	1772		ILE			45.189	41.151	23.637	1.00 24.58	•
•	MOTA	1773		ILE			46.317	42.149	23.433	1.00 26.69	
	ATOM	1774	C			295	43.720	39.636	25.717	1.00 24.80	
	ATOM	1775	0			295	44.214	39.687	26.842	1.00 25.33	
35	MOTA	1776	N			296	42.539	40.173	25.425	1.00 26.80	
	MOTA	1777	CA			296	41.743	40.853	26.444 25.894	1.00 20.30	
	ATOM	1778	CB			296	41.178	42.170	25.413	1.00 27.33	
	ATOM	1779	CG			296 296	42.240	43.141	24.826	1.00 35.56	
40	MOTA	1780	CD				41.634	45.283	25.900	1.00 39.29	
40	MOTA	1781	CE			296	41.009	46.603	25.357	1.00 33.23	
	ATOM	1782	NZ			296 296	40.564	39.958	26.893	1.00 25.50	
	ATOM	1783	C			296	 39.770	40.361	27.713	1.00 24.02	_
	ATOM	1784	И О			296 297	40.550	38.742		1.00 25.67	
15	MOTA	1785				297	39.500	37.777	26.666	1.00 25.16	_
45	ATOM	1786	CA CB			297	39.632	37.285	28.111	1.00 24.80	
	ATOM	1787	CG			297	38.766	36.068	28.460	1.00 26.43	
	MOTA	1788		LEU			39.238	34.852	27.646	1.00 26.70	
	ATOM	1789 1790		LEU			38.856	35.777	29.951	1.00 24.84	
60	ATOM		CDZ			297	38.151	38.459	26.467	1.00 25.13	
50	ATOM	1791 1792	0			297	37.261	38.378	27.309	1.00 25.28	
	ATOM	1792	N			298	38.007	39.127	25.331	1.00 24.98	
	ATOM ATOM	1793	CA			298	36.786	39.847	25.023	1.00 25.3	
	ATOM	1794	CB			298	37.143	41.139	24.291	1.00 27.13	
55	ATOM	1796	CG			298	35.991	42.092	24.108	1.00 31.28	
رر	ATOM	1797	CD			298	36.419	43.362	23.410	1.00 34.40	
	ATOM	1798		. GLU			37.348	44.027	23.918	1.00 35.9	
	MOTA	1799	-	GLU			35.832	43.693	22.359	1.00 36.10	
	MOTA	1800	C			298	35.766	39.057	24.207	1.00 23.7	
	A-011	~ ~ ~ ~	_								

	ATOM	1801	0	GLU	Α	298	:	35.	832	39.	.017	22	.979	1.	00	24.35	A
	MOTA	1802	N	TYR	A	299	:	34.	825	38	427	24	.902	1.	00	23.45	A
	ATOM	1803	CA	TYR	Α	299		33.	760	37	. 663	24	.265	1.	00	23.98	A
	ATOM	1804	CB	TYR	Α	299	:	34.	264	36	.304	23	.755	1.	00	20.13	A
5	MOTA	1805	CG	TYR	A	299	;	34.	348	35	. 233	24	.828	1.	00	21.17	A
	MOTA	1806	CD1	TYR	A	299	:	35.	.336	35	.279	25	.810	1.	00	19.32	Α
	MOTA	1807	CE1	TYR	A	299		35.	.389	34	.332	26	.826	1.	00	19.30	A
	ATOM	1808	CD2	TYR	A	299		33.	410	34	.201	24	.888	1.	.00	18.96	A
	MOTA	1809	CE2	TYR	A	299	;	33.	.456	33	.243	25	.907			19.41	A
10	MOTA	1810	CZ	TYR	Α	299	•	34.	.449	33	.321	26	.870			18.79	A
	MOTA	1811	OH	TYR	Α	299	;	34.	.511	32	.401	27	.881			18.77	Α
	MOTA	1812	С	TYR	Α	299	;	32.	. 699	37	.437	25	.331			25.20	A
	MOTA	1813	0	TYR	Α	299		32.	.942	37	.681	26	.506			26.46	A
	ATOM	1814	N	ASP	Α	300		31	.522	36	.981	24	.927			26.94	A
15	ATOM	1815	CA	ASP	A	300		30	.467	36	.710	25	.891			30.60	A
	ATOM	1816	CB	ASP	A	300		29	.665	37	.981	26	.179			35.86	A
	ATOM	1817	CG	ASP	A	300		29	.228	38	.687	24	.923			42.04	A
	ATOM	1818	OD1	ASP	Α	300		28	.450	38	.088	24	.149			45.98	A
	MOTA	1819	OD2	ASP	Α	300		29	.666	39	.840	24	.707			45.69	Α
20	MOTA	1820	C	ASP	Α	300		29	.564	35	.608	25	.363			29.26	A
	MOTA	1821	0	ASP	A	300		29	.590	35	.299		.172			28.64	A
	MOTA	1822	N	PHE	A	301		28	.778	35	.011		.253			28.96	A
	MOTA	1823	CA	PHE	A	301		27	.884	33	. 924		.871			30.48	Α
	MOTA	1824	CB	PHE	A	301		27	.818	32	. 854		.968			29.17	A
25	MOTA	1825	CG	PHE	A	301		29	.147		.279		.356			29.29	A
	MOTA	1826	CD1	PHE	A	301			.978		. 949		.245			27.31	Α
	ATOM	1827	CD2	PHE	Α	301		29	.560	31	.050		.845			27.89	A
	MOTA	1828	CE1	PHE	Α	301		31	.205	32	.403		.625			28.83	A
	MOTA	1829	CE2	PHE	Α	301			.781		.498		.217			28.05	A
30	MOTA	1830	CZ	PHE					.605		.175		.110			28.27	A
	MOTA	1831	G.	PHE					.459		.384		.619			32.20	A
	MOTA	1832				301			.946		.261		.317			32.36	A
	MOTA	1833	N			302			.798		.804		.607			33.29	A
	ATOM	1834	CD			302			.313		.943		.529			34.04	A
35	MOTA	1835	CA			302			.415		.199		.341			35.24	A
	ATOM	1836	CB			302			.144		.608		.959			34.01	A
	MOTA	1837	CG			302			.041		.413		.921			35.48	A
	MOTA	1838	C			302			.567		.561		.444			37.39	A
	MOTA	1839	0			302			.935		.518		.986			38.49	A
40	ATOM	1840	N			303			.447		.188		783			39.36	A
	MOTA	1841	CA			303			.572		.692		843			40.65	A
	MOTA	1842	CB			303			.280		.506		.862			41.66	A A
	MOTA	1843	C	-		303			.238		.197		814			41.25	A
	MOTA	1844	0			303			.253		.537		1.854			43.16 41.04	A
45	MOTA	1845	N			304			.945		.665		6.631			40.66	A
	MOTA	1846	CA			304			.569		.258		.480			41.36	A
	MOTA	1847	CB			304			.121		.004		.040			39.61	Ā
	MOTA	1848	C			304			.628		.223		5.876 5.395			40.61	A
50	ATOM	1849	0			304			.298		.156 .543		5.617			36.21	A
50	MOTA	1850	N			305			.891		.662					32.08	A
	ATOM	1851	CA			305			.022		.519		5.909 5.187			29.46	Α
	MOTA	1852	CB			305			.259		.917					28.15	Α
	MOTA	1853	CG			305			.536		.875		5.690 5.377			26.20	A
E E	MOTA	1854		PHE					.146		.386		1.521			27.05	A
55	ATOM	1855		PHE					.127		.308		5.908			26.92	A
	MOTA	1856		PHE					.330		.826		1.042			26.62	A
	MOTA	1857	CEZ			305			.914		.786		1.737			26.61	A
	MOTA	1858	C			305			.811		.664		. 13 i 7 . 057			30.09	Α
	MOTA	1859	C	FRE	A	303		د 2		۷.		2		_			

	MOTA	1860	0	PHE	A	305	23.	518	28.051	28.187		31.51	Α.
	MOTA	1861	N	PHE	Α	306	23.		26.378	26.758		27.01	A
)	ATOM	1862	CA	PHE	A	306	23.	801	25.334	27.769		26.30	A
	ATOM	1863	CB	$_{ m PHE}$	A	306	24.	157	23.970	27.170	1.00	25.03	A
5	MOTA	1864	CG	PHE	Α	306	23.	548	23.725	25.815	1.00	27.24	A
	MOTA	1865	CD1	PHE	Α	306	22.	170	23.831	25.622	1.00	28.40	A
	MOTA	1866	CD2	PHE	A	306	24.	350	23.386	24.728	1.00	27.84	A
	ATOM	1867	CE1	PHE	A	306	21.	601	23.603	24.365	1.00	28.05	A
	ATOM	1868	CE2	PHE	А	306	23.	792	23.155	23.465	1.00	28.31	A
10	ATOM	1869	CZ	PHE			22.	415	23.263	23.283	1.00	28.00	A
	ATOM	1870	C	PHE			24.	711	25.652	28.961	1.00	26.23	A
	ATOM	1871	Ö,	PHE			25.		25.775	28.811	1.00	25.59	A
	ATOM	1872	N	PRO			24.		25.796	30.163	1.00	26.67	A
	MOTA	1873	CD	PRO			22.		25.625	30.430	1.00	27.95	A
15	ATOM	1874	CA	PRO			24.		26.110	31.405		26.59	A
1.5	ATOM	1875	CB	PRO				795	25.832	32.481		26.14	A
	ATOM	1876	CG	PRO			22.		26.250	31.803		27.86	A
	ATOM	1877	C	PRO			26.		25.355	31.659		25.58	A
	ATOM	1878	0	PRO				189	25.964	31.900		22.65	A
20	ATOM		N	LYS				085	24.031	31.620		24.46	A
20			CA.	LYS				274	23.232	31.867		23.91	A
	MOTA	1880						887	21.760	32.024		23.25	A
	ATOM	1881	CB	LYS					21.700	33.285		28.49	A
	ATOM	1882	CG	LYS				062	20.093	33.466		30.17	A
25	ATOM	1883	CD	LYS			25.			34.722		33.12	À
25	MOTA	1884	CE	LYS				760	19.973	34.722		34.13	A
	MOTA	1885	NZ	LYS				122	18.636				
	MOTA	1886	C	LYS				314	23.426	30.769		22.84	A
	MOTA	1887	.0	LYS				514	23.411	31.042		22.46	A
	MOTA	1888	N	ALA				861	23.621	29.534		21.59	A
30	ATOM	1889	CA	ALA				792	23.848	28.432		20.02	A
	ATOM	1890	CB	ALA				056	23.856	27.106		18.80	Α.
	ATOM	1891	C	ALA				481	25.191	28.662		21.41	A
	ATOM	1892	0	ALA				680	25.335	28.427		21.39	A
	ATOM	1893	N	ARG				717	26.179	29.121		21.39	A
35	ATOM	1894	CA	ARG				290	27.494	29.388		22.02	A
	ATOM	1895	CB	ARG				213	28.479	29.854		22.39	A
-	ATOM	1896	CG	ARG				806	29.756	30.436		25.30	A
	ATOM	1897	CD	ARG				780	30.852	30.664		28.33	A
	ATOM	1898	NE	ARG				420	32.039	31.230		30.18	A
40	ATOM .	1899	CZ	ARG				901	33.263	31.203		32.07	A
	MOTA	1900		ARG				719	33.477	30.634		31.19	A
	MOTA	1901	NH2					567	34.277	31.742		30.49	A
	ATOM	1902	C	ARG				376	27.388	30.458		21.65	A
	ATOM	1903	0	ARG				464	27.949	30.311		20.36	A
45 ,	ATOM	1904	N	ASP				074	26.677	31.541		19.57	A
	MOTA	1905	CA	ASP	Α	311		043	26.512	32.615		20.18	A
	ATOM	1906	CB			311		460	25.649	33.739		20.39	A
	MOTA	1907	CG	ASP				439	25.446	34.881		23.35	A
	MOTA	1908		ASP				158	24.428	34.885		24.91	A
50	ATOM	1909	OD2	ASP	Α	311	31.	500	26.312	35.776		26.96	Α
	MOTA	1910	C	ASP				322	25.877	32.073		19.73	A
	MOTA	1911	0	ASP	Α	311		422	26.289	32.439		19.30	Α.
	MOTA	1912	N			312		179	24.891	31.188		16.32	A
	MOTA	1913	CA	LEU				349	24.226	30.611		16.66	A
55	ATOM	1914	CB			312		927	23.035	29.744		16.12	A.
	ATOM	1915	CG	LEU				050	22.320	28.974		14.73	A
	MOTA	1916		LEU				192	21.935	29.912		14.56	A
	MOTA	1917	CD2	LEU	A	312		477	21.084	28.289		14.22	A
	MOTA	1918	С	LEU	A	312	34.	181	25.189	29.774	1.00	16.61	A

	ATOM	1919	0	LEU 2	A 312		35.402	25.241	29.910	1.00	16.20	A
	ATOM	1920	N	VAL 2	A 313		33.515	25.949	28.908	1.00	L6.20	A
	ATOM	1921	CA	VAL	A 313		34.207	26.907	28.058	1.00	L5.37	A
	ATOM	1922	CB		A 313		33.216	27.648	27.130	1.00	L6.42	A
5	ATOM	1923		VAL			33.915	28.796	26.426	1.00	16.93	A
_	ATOM	1924		VAL			32.644	26.672	26.103	1.00	L7.88	·A
	ATOM	1925	C		A 313		34.960	27.923	28.911	1.00	17.39	A
	ATOM	1926	0		A 313		36.093	28.294	28.591	1.00	18.00	A
	ATOM	1927	И		A 314		34.342	28.364	30.004	1.00	17.61	A
10	ATOM	1928	CA		A 314		34.986	29.331	30.885	1.00 2		A
10	ATOM	1929	CB		A 314		34.009	29.816	31.959	1.00 2		A
		1930	CG		A 314		32.800	30.550	31.396	1.00 2		· A
	ATOM	1931	CD		A 314		31.852	31.025	32.478	1.00		A
	ATOM	1931		GLU .			31.580	30.246	33.417	1.00		A
15	MOTA		OE2		A 314		31.370	32.173	32.387	1.00		A
15	ATOM	1933					36.217	28.721	31.539	1.00		A
	MOTA	1934	C		A 314 A 314		37.134	29.433	31.934	1.00		A
	ATOM	1935	0				36.245	27.400	31.651	1.00		A
	ATOM	1936	N		A 315	•	37.394	26.749	32.258	1.00		A
20	ATOM	1937	CA		A 315		36.946	25.514	33.043	1.00		A
20	ATOM	1938	CB		A 315			25.885	34.368	1.00		A
	ATOM	1939	CG		A 315		36.280		35.073	1.00		A
•	ATOM	1940	CD		A 315		35.653	24.696 25.095	36.427	1.00		A
	MOTA	1941	CE		A 315		35.070		37.381	1.00		A
	MOTA	1942	ΝZ		A 315		36.119	25.552	31.218	1.00		A
25	ATOM	1943	C		A 315		38.452	26.393	31.561	1.00		A
	ATOM	1944	0		A 315		39.511	25.873 26.691	29.950	1.00		A
	ATOM	1945	N		A 316		38.164	26.429		1.00		A
	ATOM	1946	CA		A 316		39.102		28.854 27.738	1.00		A
	ATOM	1947	CB		A 316		38.414	25.636		1.00		A
30	MOTA	1948	CG		A 316		38.028	24.201	28.115	1.00		A
	ATOM	1949			A 316		37.139	23.597	27.031	1.00		A
	MOTA	1950			A 316		39.302	23.373	28.309	1.00		A
	ATOM	1951	C		A 316		39.652	27.743	28.290	1.00		A
	MOTA	1952	0		A 316		40.851	27.860	28.023			A
35	ATOM	1953	N		A 317		38.780	28.729	28.105	1.00		A
	ATOM	1954	CA		A 317		39.228	30.022	27.596	1.00		A
	ATOM	1955	CB		A 317		38.083	30.752	26.887	1.00		A
	ATOM	1956	CG		A 317		37.448	29.973	25.727	1.00		A
	MOTA	1957			A 317		36.415	30.851	25.018			
40	ATOM -	1958			A 317		38.528	29.526	24.741	1.00		A
	MOTA	1959	С		A 317		39.745	30.841	28.774	1.00		A N
	MOTA	1960	.0		A 317		39.078	31.753	29.273		18.58	A A
•	MOTA	1961	N		A 318		40.937	30.475	29.229	1.00		A
	ATOM	1962	CA		A 318		41.593	31.141	30.342		18.85	A
45	ATOM	1963	CB		A 318		41.846	30.153	31.500	1.00		A
	MOTA	1964			A 318		42.590	30.848	32.634	1.00		A
	ATOM	1965			A 318		40.520	29.584	31.990		19.44	· A
•	MOTA	1966	C		A 318		42.923	31.657	29.811		19.67	A
	MOTA	1967	0		A 318		43.690	30.902	29.208		18.26	
50	MOTA	1968	N		A 319		43.197	32.939	30.028		20.07 20.98	A A
	MOTA	1969	CA		A 319		44.436	33.533	29.538			A
	MOTA	1970	CB		A 319		44.521	35.002	29.968		21.64	A
	ATOM	1971	CG		A 319		43.418	35.908	29.408		24.38	A A
_	MOTA	1972			A 319		43.606	37.332	29.935		23.28	A
55	MOTA	1973			A 319		43.453	35.887	27.875		24.33	A
	MOTA	1974	C		A 319		45.680	32.774	29.994		20.38 21.34	A
	MOTA	1975	0		A 319		46.568	32.496	29.192		20.22	. A
	ATOM	1976	N		A 320		45.742	32.440	31.280			A
	MOTA	1977	CA	ASP	A 320		46.879	31.707	31.833	1.00	20.90	r.

	ATOM	1978	СВ	ASP	A	320	4	6.84	2	31.760	33.365		20.76	A
٠.	MOTA	1979	CG	ASP	A	320	4	8.04	9	31.102	34.004	1.00	21.51	A
	MOTA	1980	OD1	ASP	A	320	4	8.66	9	30.226	33.367	1.00	23.46	A
	MOTA	1981	OD2	ASP	Α	320	. 4	8.37	1	31.450	35.159	1.00	23.89	A
5	MOTA	1982	С	ASP	A	320	4	6.81	4	30.247	31.367		20.06	A
	MOTA	1983	0	ASP	Α	320	4	5.98	8	29.476	31.840	1.00	20.54	A
	MOTA	1984	N	ALA	Α	321	4	7.70	0	29.876	30.451		20.68	A
	MOTA	1985	CA	ALA	Α	321	4	7.73	3	28.522	29.903		22.04	A
	MOTA	1986	CB	ALA	A	321	4	8.86	0	28.411	28.881		20.75	A
10	MOTA	1987	C	ALA	A	321	4	7.85	8	27.400	30.940		21.62	A
	MOTA	1988	0	ALA	A	321	4	7.48	2	26.259	30.665		21.99	A
	MOTA	1989	N	THR				8.37		27.715	32.127		20.89	A
	MOTA	1990	CA	THR				8.53		26.698	33.167		20.82	A
	MOTA	1991	CB	THR				9.67		27.051	34.146		19.47	A
15	MOTA	1992		THR				9.34		28.253	34.848		20.19	A
	ATOM	1993	CG2	THR				0.98		27.249	33.394		21.59	A
	ATOM	1994	С	THR				7.26		26.498	33.983		19.55	· A
	MOTA	1995	0	THR				7.23		25.673	34.894		21.13	A
	MOTA	1996	N	LYS				6.21		27.248	33.661		19.33	A
20	MOTA	1997	CA	LYS				4.96		27.122	34.392		21.20	A A
	ATOM	1998	CB	LYS				4.58		28.460	35.030		23.75	A
	ATOM	1999	CG	LYS				15.56		28.933	36.084		28.45 33.76	A
	ATOM	2000	CD	LYS				15.05		30.177	36.799 37.802		36.15	A
25	MOTA	2001	CE	LYS				16.08		30.678			37.34	A
25	MOTA	2002	NZ	LYS				16.53 13.80		29.569 26.614	38.693 33.539		20.68	A
	MOTA	2003 2004	С 0	LYS				12.64		26.757	33.915		20.42	A
	ATOM ATOM	2004	N	ARG				4.11		26.019	32.392		19.97	A
	MOTA	2005	CA	ARG				13.06		25.494	31.531		17.98	A
30	MOTA	2007	CB	ARG				13.46		25.609	30.061		15.95	A
50	ATOM	2008	CG	ARG				13.53		27.050	29.603		17.34	
	MOTA	2009	CD	ARG				13.99		27.194	28.172		19.80	A
	MOTA	2010	NE	ARG				4.43		28.565	27.944		16.93	A
	ATOM	2011	CZ	ARG				15.41		28.908	27.108		19.88	Α
35	ATOM	2012		ARG				6.04		27.978	26.398	1.00	14.58	Α.
	MOTA	2013		ARG				15.77		30.181	27.015	1.00	16.51	A
	ATOM	2014	С	ARG	Α	324	4	12.76	2	24.046	31.883	1.00	18.32	A
	ATOM	2015	0	ARG	A	324	4	13.67	3	23.222	32.006	1.00	18.20	A
	MOTA	2016	N	LEU	Α	325	4	11.47	9	23.748	32.055	1.00	18.32	A
40	MOTA	2017	CA	LEU	Α	325	4	11.05	0	22.403	32.395	1.00	17.79	A
	MOTA	2018	CB	LEU	A	325		39.52	:3	22.335	32.425	1.00	17.03	A
	ATOM	2019	CG	LEU	A	325	:	38.89	6	21.125	33.116	1.00	15.91	A
	MOTA	2020	CD1	LEU	А	325	:	39.39	2	21.048	34.557	1.00	15.93	A
	MOTA	2021	CD2	LEU				37.37		21.255	33.084		16.56	A
45	MOTA	2022	С	PE O	Α	325	4	11.59	9	21.433	31.356		18.68	A
	MOTA	2023	0	LEU	A	325	4	11.34	7	21.586	30.157		18.28	A
	MOTA	2024	N			326		12.35		20.439	31.821		18.18	A
	MOTA	2025	CA			326		12.93		19.462	30.915		16.36	A
	ATOM	2026	С			326		14.44		19.558	30.807		19.15	A
50	ATOM	2027	0			326		15.09		18.592	30.404		19.52	A
	ATOM	2028	И	CYS				15.01		20.708	31.161		18.16	A
	MOTA	2029	CA			327		16.46		20.867	31.075		19.30	A N
	ATOM	2030	CB			327		46.85		22.350	31.058		20.22 21.97	A A
	MOTA	2031	SG			327		16.78		23.200	32.649		20.22	A
55	ATOM	2032	C			327		47.16		20.157	32.228 33.246		17.92	A
	ATOM	2033	0			327		16.56		19.828 19.933	32.053		20.51	Ā
	ATOM ATOM	2034 2035	N CA			328 328		48.46 49.27		19.244	33.042		23.34	A
	ATOM	2035	CB			328		19.27 50.71		19.139	32.507		28.68	A
	111 Old	2030	<u> </u>	0110	~			JU - 1 A			52.50.			

	MOTA	2037	CG	GLU	A	328	50.754	18.367	31.175	1.00 38.24	A
	ATOM	2038	CD	GLU	Α	328	52.067	18.500	30.414	1.00 43.23	A
	ATOM	2039	OE1	GLU	Α	328	52.535	19.643	30.218	1.00 46.22	A
	MOTA	2040	OE2	GLU	А	328	52.618	17.459	29.991	1.00 44.90	A
5	MOTA	2041	С	GLU	А	328	49.234	19.876	34.435	1.00 22.11	A
	ATOM	2042	0	GLU	A	328	49.147	19.161	35.437	1.00 -20.27	A
	MOTA	2043	N	GLU	Α	329	49.276	21.204	34.506	1.00 18.40	A
	MOTA	2044	CA	GLU	Α	329	49.248	21.875	35.801	1.00 20.13	A
	ATOM	2045	CB	GLU	Α	329	49.587	23.363	35.657	1.00 20.36	A
10	ATOM	2046	CG	GLU	А	329	51.014	23.651	35.190	1.00 24.05	A
	ATOM	2047	CD	GLU	Α	329	51.191	23.518	33.688	1.00 25.93	A
	MOTA	2048	OE1	GLU	Α	329	50.213	23.154	32.995	1.00 26.61	A
	MOTA	2049	OE2	GLU	Α	329	52.311	23.781	33.198	1.00 27.19	A
-	MOTA	2050	С	GLU	Α	329	47.890	21.718	36.480	1.00 19.36	A
15	MOTA	2051	0	GLU	A	329	47.775	21.879	37.694	1.00 18.74	. А
	ATOM	2052	N	MET	Α	330	46.863	21.415	35.691	1.00 17.28	A
	ATOM	2053	CA	MET	Α	330	45.520	21.220	36.229	1.00 16.38	A
	ATOM	2054	CB	MET	Α	330	44.474	21.833	35.294	1.00 17.65	A
	ATOM	2055	CG	MET	A	330	44.460	23.365	35.311	1.00 22.95	A
20	MOTA	2056	SD	MET	A	330	44.186	24.026	36.979	1.00 26.78	A
	MOTA	2057	CE	MET	A	330	42.435	23.712	37.186	1.00 24.69	A
	MOTA	2058	C	MET			45.257	19.730	36.422	1.00 14.30	A
	ATOM	2059	0	MET	Α	330	44.127	19.304	36.629	1.00 15.39	A
	ATOM	2060	N	GLU	Α	331	46.327	18.949	36.346	1.00 15.60	A
25	MOTA	2061	CA	GLU	Α	331	46.289	17.501	36.531	1.00 17.08	A
	MOTA	2062	CB	GLU	Α	331	45.607	17.155	37.862	1.00 17.00	A
	MOTA	2063	CG	GLU	Α	331	46.070	18.027	39.038	1.00 17.46	A
	MOTA	2064	CD	GLU	A	331.	47.591	18.179	39.145	1.00 20.16	A
	MOTA	2065	OE1	GLU	Α	331	48.034	19.073	39.896	1.00 21.39	A
30	MOTA	2066	OE2	GLU	Α	331	48.345	17.420	38.500	1.00 18.87	A
	MOTA	2067	С	GLU	Α	331	45.697	16.658	35.398	1.00 17.80	A
	MOTA	2068	0	GLU	Α	331	45.107	15.602	35.636	1.00 20.40	A
	MOTA	2069	N	GLY	A	332	45.844	17.133	34.167	1.00 16.23	A
•	MOTA	2070	CA	GLY	А	332	45.420	16.353	33.015	1.00 14.10	A
35	MOTA	2071	C	GLY			43.982		32.596	1.00 13.54	. A
	ATOM	2072	0			332	43.063	16.864	33.017	1.00 11.96	A
	MOTA	2073	N			333	43.804	15.141	31.750	1.00 14.37	A
	MOTA	2074	CA			333	42.510	14.806	31.182	1.00 13.56	A
	ATOM	2075	СВ			333	42.722	13.892	29.968	1.00 15.00	A
40 ·	ATOM	2076	CG			333	43.153	14.683	28.752	1.00 16.46	A
	MOTA	2077		TYR			42.206	15.172	27.849	1.00 15.29	A
	ATOM	2078		TYR			42.573	16.002	26.794	1.00 13.42	A
	ATOM	2079		TYR			44.490	15.039	28.561	1.00 14.91	A
	ATOM	2080		TYR			44.872	15.877	27.499	1.00 14.87	A
45	ATOM	2081	CZ	TYR			43.902	16.353	26.626	1.00 15.61	A
	ATOM	2082	ОН			333	44.244	17.197	25.599	1.00 17.29	A
	ATOM	2083	С			333	41.470	14.230	32.127	1.00 15.23	A
	ATOM	2084	0			333	40.278	14.323	31.846	1.00 16.63	A
	MOTA	2085	N			334	41.907	13.650	33.244	1.00 15.50	A
50	ATOM	2086	CA			334		13.100	34.202	1.00 15.07	A
	ATOM	2087	C			334	39.925	14.146	34.616	1.00 16.40	A
	ATOM	2088	0			334	38.724	13.946	34.433	1.00 15.05	A
	MOTA	2089	И			335	40.366	15.278	35.184	1.00 14.96	A.
<i>E E</i>	ATOM	2090	CD			335	41.727	15.531	35.689	1.00 15.88 1.00 15.29	A A
55	ATOM	2091	CA			335 335	39.444	16.339	35.606	1.00 15.29	A
	ATOM	2092	CB				40.383	17.397	36.178	1.00 13.19	A
	ATOM	2093	CG			335	41.485	16.569	36.758	1.00 15.81	A
	ATOM	2094	C			335	38.594	16.877	34.448	1.00 15.84	A
	MOTA	2095	0	PRO	А	335	37.423	17.204	34.631	1.00 T4.04	~

	ATOM	2096	N	LEU	A	336	39.184	16.971	.33.257	1.00 16.12	A
	ATOM	2097	CA	LEU	Α	336	38.450	17.465	32.094	1.00 15.52	A
	ATOM	2098	CB	LEU	Α	336	39.396	17.653	30.898	1.00 14.39	A
	ATOM	2099	CG	LEU	Α	336	38.770	17.991	29,538	1.00 15.46	A
5	ATOM	2100	CD1	LEU	Α	336	37.836	19.182	29.662	1.00 11.25	A
	ATOM	2101	CD2	LEU	Α	336	39.884	18.285	28.528	1.00 14.11	A
	ATOM	2102	С	LEU	Α	336	37.321	16.508	31.714	1.00 16.28	A
	ATOM	2103	0	LEU	Α	336	36.176	16.921	31.540	1.00 15.51	A
	ATOM	2104	N	LYS	Α	337	37.640	15.225	31.592	1.00 17.22	A
10	ATOM	2105	CA	LYS	Α	337	36.624	14.243	31.235	1.00 17.39	A
	MOTA	2106	CB	LYS	Α	337	37.293	12.900	30.921	1.00 17.68	A
	ATOM	2107	CG	LYS	A	337	38.170	12.994	29.676	1.00 22.31	A
	ATOM	2108	CD	LYS	Α	337	39.213	11.892	29.592	1.00 24.60	A
	ATOM	2109	CE	LYS	Α	337	38.620	10.560	29.189	1.00 24.76	A
15	ATOM	2110	NZ	LYS	Α	337	39.710	9.560	28.997	1.00 25.05	Α
	ATOM	2111	С	LYS	Α	337	35.577	14.096	32.342	1.00 17.33	A
	ATOM	2112	0	LYS			34.456	13.652	32.090	1.00 14.42	A
	ATOM	2113	N	ALA	Α	338	35.928	14.500	33.559	1.00 15.83	A
	ATOM	2114	CA	ALA	Α	338	34.989	14.395	34.674	1.00 17.52	A
20	ATOM	2115	CB	ALA	Α	338	35.749	14.167	35.980	1.00 19.68	A
	ATOM	2116	C	ALA			34.095	15.621	34.804	1.00 18.83	A
	ATOM	2117	0	ALA			33.252	15.687	35.695	1.00 18.94	A
	ATOM	2118	N	HIS			34.262	16.596	33.918	1.00 19.42	A
	ATOM	2119	CA	HIS			33.438	17.796	34.004	1.00 19.28	A
25	ATOM	2120	CB			339	33.865	18.819	32.949	1.00 19.20	A
	ATOM	2121	CG	HIS	Α	339	33.163	20.134	33.074	1.00 20.26	A
	ATOM	2122		HIS			33.549	21.299	33.649	1.00 18.95	A
	MOTA	2123	ND1	HIS	Α	339	31.880	20.340	32.612	1.00 19.10	A
	ATOM	2124	CE1	HIS	A	339	31.506	21.576	32.896	1.00 22.19	A
30	MOTA	2125	NE2	HIS	Α	339	32.500	22.179	33.525	1.00 21.98	A
	ATOM	2126	C	HIS	A	339	31.957	17.448	33.845	1.00 19.13	A
	MOTA	2127	0	HIS	Α	339.	31.597	16.576	33.061	1.00 19.52	Α
•	ATOM	2128	N	PRO	Α	340	31.079	18.125	34.606	1.00 19.80	Α
	ATOM	2129	CD	PRO	A	340	31.424	19.119	35.640	1.00 19.08	A
35	ATOM	2130	CA	PRO	Α	340	29.630	17.900	34.569	1.00 20.52	A
	ATOM	2131	CB	PRO	Α	340	29.091	19.058	35.396	1.00 20.74	A
	ATOM	2132	CG	PRO	Α	340	30.146	19.207	36.454	1.00 19.20	Α
	MOTA	2133	С	PRO	A	340	29.000	17.834	33.176	1.00 21.42	A
	MOTA	2134	0	PRO	Α	340	28.049	17.088	32.955	1.00 22.48	. А
40	ATOM	2135	N	PHE	Α	341	29.528	18.606	32.237	1.00 21.33	A
	ATOM	2136	CA	PHE	Α	341	28.985	18.610	30.886	1.00 21.57	A
	ATOM	2137	CB	PHE	Α	341	29.739	19.624	30.017	1.00 21.64	A
	ATOM	2138	CG	PHE	Α	341	29.207	19.740	28.613	1.00 23.18	A
	ATOM	2139	CD1	PHE	A	341	27.903	20.171	28.382	1.00 22.58	Α
45	MOTA	2140	CD2	PHE	Α	341	30.013	19.431	27.522	1.00 21.95	A
	MOTA	2141	CE1	PHE	Α	341	27.410	20.292	27.082	1.00 23.54	A
	ATOM	2142	CE2	PHE	Α	341	29.533	19.548	26.220	1.00 21.83	A
	ATOM	2143	cz	PHE	A	341	28.228	.19.980	25.998	1.00 23.23	A
	MOTA	2144	C	PHE	Α	341	29.055	17.226	30.237	1.00 21.84	A
50	MOTA	2145	0			341	28.232	16.896	29.389	1.00 20.37	A
	ATOM	2146	N			342	30.034	16.422	30.640	1.00 20.51	A
	MOTA	2147	CA	PHE	A	342	30.221	15.085	30.077	1.00 23.01	Α
	MOTA	2148	CB			342	31.710	14.809	29.850	1.00 18.00	A
	MOTA	2149	CG	, bhe			32.398	15.812	28.971	1.00 17.05	A
55	MOTA	2150		PHE			32.010	15.987	27.652	1.00 17.78	A
	MOTA	2151		PHE			33.487	16.534	29.450	1.00 15.72	A
•	ATOM ·	2152		PHE			32.702	16.867	26.811	1.00 18.08	A
	MOTA	2153		PHE			34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ	PHE	A	342	33.790	17.578	27.298	1.00 16.56	A

	ATOM .	2155	C	PHE 2	A 342	29.679	13.972	30.976	1.00 24.95	A
	ATOM	2156	0	PHE 2	A 342	30.002	12.798	30.777	1.00 23.95	A
	MOTA	2157	N	GLU I	A 343	28.861	14.333	31.958	1.00 27.35	A
	MOTA	2158	CA	GLU 2	A 343	28.325	13.349	32.897	1.00 30.28	A
5	MOTA	2159	CB	GLU I	A 343	27.187	13.964	33.716	1.00 32.20	A
	MOTA	2160	ÇG	GLU	A 343	26.581	12.991	34.714	1.00 39.71	A
	ATOM	2161	CD	GLU	A 343	25.628	13.661	35.688	1.00 44.72	A
	ATOM	2162	OE1	GLU	A 343	24.661	14.314	35.234	1.00 47.55	A
	MOTA	2163	OE2	GLU	A 343	25.847	13.526	36.911	1.00 46.89	A
10	ATOM	2164	С	GLU	A 343	27.852	12.017	32.305	1.00 28.98	A
	MOTA	2165	0	GLU	A 343	28.225	10.952	32.800	1.00 31.73	A
	ATOM	2166	N	SER :	A 344	27.037	12.067	31.258	1.00 26.09	A
	MOTA	2167	CA	SER :	A 344	26.520	10.838	30.656	1.00 28.36	A
	MOTA	2168	CB	SER :	A 344	25.129	11.089	30.067	1.00 28.73	· A
15	ATOM	2169	QG	SER .	A 344	25.203	11.942	28.940	1.00 30.91	A
	ATOM	2170	C	SER .	A 344	27.407	10.214	29.577	1.00 27.66	A
	MOTA	2171	0	SER .	A 344	26.987	9.281	28.900	1.00 28.66	A
	MOTA	2172	N	VAL .	A 345	28.627	10.715	29.419	1.00 26.75	A
	ATOM	2173	CA	VAL .	A 345	29.534	10.183	28.402	1.00 23.44	A
20	MOTA	2174	CB	VAL .	A 345	30.565	11.256	27.950	1.00 23.10	A
	MOTA	2175	CG1	VAL .	A 345	31.589	10.631	26.995	1.00 22.24	A
	MOTA	217.6	CG2	VAL .	A 345	29.854	12.418	27.275	1.00 20.05	A
	ATOM	2177	С	VAL .	A 345	30.326		28.855	1.00 24.26	A
	ATOM	. 2178	0	VAL	A 345	30.876	8.930	29.960	1.00 22.83	A
25	MOTA	2179	N	THR	A 346	30.374	7.942	27.997	1.00 21.77	A
	MOTA	2180	CA	THR	A 346	31.153	6.740	28.272	1.00 23.70	A
	MOTA	2181	CB	THR	A 346	30.391	5.455	27.857	1.00 26.53	A .
	MOTA	2182	OG1	THR	A 346	5 29.248	5.284	28.706	100 29.98	A
	MOTA	2183	CG2	THR	A 346	31.289	4.231	27.990	1.00 24.28	A
30	ATOM	2184	С	THR	A 346	32.383	6.945	27.385	1.00 23.43	A
	MOTA	2185	0	THR	A 346	32.306	6.827	26.160	1.00 24.50	A
	MOTA	2186	N	TRP	A 347	7 33.508	7.27,0	28.013	1.00 22.98	A
	ATOM	2187	CA	TRP	A 347	34.744	7.569	27.300	1.00 23.81	A
	MOTA	2188	CB	TRP	A 347	7 35.683	8.352	28.219	1.00 22.54	A
35	ATOM	2189	CG	TRP	A 347	7 35.128	9.658	28.693	1.00 20.61	A
-	ATOM	2190	CD2	TRP	A 347	7 35.257	10.927	28.040	1.00 19.11	A
	MOTA	2191	CE2	TRP	A 34'	7 34.581	11.881	28.838	1.00 18.39	A
	MOTA	2192	CE3	TRP	A 34	7 35.878		26.858	1.00 18.16	A
	MOTA	2193	CD1	TRP	A 34'	7 34.397		29.828	1.00 18.35	A
40	MOTA	2194	NE1	TRP				29.923	1.00 19.51	A
	ATOM	2195	CZ2		A 34'			28.491	1.00 16.88	A
	MOTA	2196	CZ3		A 34'			26.511	1.00 17.23	. A
	MOTA	2197	CH2		A 34'			27.327	1.00 18.16	A
	ATOM	2198	С	TRP	A 34'	7 35.538	6.429	26.675	1.00 25.79	A
45	ATOM	2199	0		A 34'			25.742	1.00 24.67	A
	ATOM	2200	N		A 34			27.183	1.00 27.10	A
	ATOM	2201	CA	ALA	A 34	B 36.116		26.697	1.00 27.46	A
	ATOM	2202	CB	ALA	A 34			27.636	1.00 27.09	A
	ATOM	2203	С		A 34			25.256	1.00 27.18	A
50	ATOM	2204	0	ALA	A 34	B 36.830		24.613	1.00 29.41	A
	ATOM	2205	N	ASN	A 34			24.735	1.00 26.55	A
	MOTA	2206	CA		A 34			23.375	1.00 27.28	A
	MOTA	2207	CB		A 34			23.444	1.00 29.37	A
	MOTA	2208	CG		A 34			24.013	1.00 30.92	A
55	ATOM	2209		ASN				24.859	1.00 30.17	A
	MOTA	2210		ASN		·		23.553	1.00 33.52	A
	MOTA	2211	C		A 34			22.509	1.00 26.47	A
	MOTA	2212	0		A 34			21.819	1.00 25.87	A
	MOTA	2213	N	LEU	A 35	0 33.94′	7 5.543	22.518	1.00 24.45	A

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1.00 23.14 LEU A 350 33.203 6.510 21.721 CA MOTA 2214 21.848 1.00 23.22 CB LEU A 350 33.837 7.898 MOTA 2215 1.00 21.05 A 2216 CG LEU A 350 33.659 8.605 23.191 MOTA 1.00 19.36 A 23.293 CD1 LEU A 350 34.646 9.756 MOTA 2217 23.319 1.00 18.78 Α CD2 LEU A 350 32.220 9.094 2218 MOTA 33.082 6.152 20.240 1.00 22.60 Α С LEU A 350 ATOM 2219 6.296 1.00 21.15 2220 0 LEU A 350 32.011 19.650 Α ATOM 1.00 23.13 HIS A 351 34.165 5.689 19.627 Α ATOM 2221 N 1.00 27.83 CA HIS A 351 34.089 5.387 18.204 Ά ATOM 2222 17.596 1.00 29.36 Α HIS A 351 35.506 5.325 10 **ATOM** 2223 CB 36.082 17.493 1.00 32.07 HIS A 351 3.950 2224 CG MOTA 2225 CD2 HIS A 351 36.611. 3.128 18.431 1.00 32.39 Α MOTA 16.291 1.00 33.02 Α 2226 ND1 HIS A 351 36.197 3.285 ATOM 16.493 1.00 33.58 Α 2227 CE1 HIS A 351 36.775 2.113 ATOM 37.036 17.782 1.00 31.76 Α NE2 HIS A 351 1.992 15 ATOM 2228 HIS A 351 33.258 4.144 17.874 1.00 28.12 Α С MOTA 2229 33.015 16.707 1.00 29.49 Α 0 HIS A 351 3.847 2230 ATOM 18.908 1.00 29.28 MOTA 2231 N **GLN A 352** 32.800 3.442 Α 1.00 29.67 Α 18.726 MOTA 2232 CA GLN A 352 31.963 2.255 19.694 1.00 30.56 Α GLN A 352 32.366 1.145 20 MOTA 2233 CB 1.00 30.88 CG GLN A 352 33.169 0.041 19.041 Α ATOM 2234 34.493 19.729 1.00 31.21 Α CD **GLN A 352** -0.186 ATOM 2235 1.00 30.76 Α OE1 GLN A 352 34.541 -0.450 20.928 MOTA 2236 18.971 1.00 32.30 Α MOTA 2237 NE2 GLN A 352 35.578 -0.084 GLN A 352 30.504 2.638 18.963 1.00 30.42 Α 25 ATOM 2238 C 1.00 29.01 Α 0 GLN A 352 29.595 1.831 18.770 2239 ATOM MOTA 2240 N GLN A 353 30.290 3.875 19.397 1.00 27.64 A 28.948 1.00 27:42 Α 19.652 MOTA 2241 CA GLN A 353 4.365 20.775 1.00 25.77 28.977 5.401 ATOM 2242 CB GLN A 353 30 GLN A 353 29.408 4.837 22.115 1.00 27.34 ATOM 2243 CG 29.638 5.914 23.156 1.00 27.19 Α 2244 CD GLN A 353 ATOM 23.252 1.00 28.29 Α OE1 GLN A 353 28.875 6.872 ATOM 2245 ` 30.687 23.951 1.00 28.79 Α 5.753 MOTA 2246 NE2 GLN A 353 GLN A 353 Α С 28.375 4.989 18.385 1.00 29.00 MOTA 2247 29.118 5.455 17.516 1.00 29.14 Α 35 ATOM 2248 0 GLN A 353 ATOM ' 1.00 27.31 27.053 Α 2249 N THR A 354 4.984 18.276 1.00 27.85 A 26.390 5.568 17.119 THR A 354 ATOM 2250 CA THR A 354 24.991 4.941 16.904 1.00 30.69 2251 CB MOTA OG1 THR A 354 25.132 3.532 16.665 1.00 30.07 Α MOTA 2252 A 24.289 5.585 15.709 1.00 29.58 40 MOTA 2253 CG2 THR A 354 1.00 26.85 Α 26.244 7.062 17.376 THR A 354 MOTA 2254 С 25.592 18.329 1.00 25.77 Α THR A 354 ' 7.475 ATOM 2255 0 PRO A 355 26.867 7.898 16.533 1.00 27.22 2256 N MOTA 2257 CD PRO A 355 27.792 7.588 15.431 1.00 25.89 Α MOTA 1.00 27.23 Α 45 ATOM 2258 CA PRO A 355 26.763 9.346 16.734 1.00 24.91 27.625 9.915 Α 15.609 MOTA 2259 CB PRO A 355 15.385 1.00 25.54 PRO A 355 28.643 8.838 2260 MOTA CG 9.837 16.641 1.00 28.07 PRO A 355 25.322 ATOM 2261 C Δ 24.548 9.364 15.810 1.00 27.24 2262 0 PRO A 355 MOTA Α 2263 N PRO A 356 24.941 10.792 17.500 1.00 28.28 50 MOTA 25.752 11.560 18.462 1.00 28.31 Α MOTA 2264 CD PRO A 356 2265 17.448 1.00 28.44 23.572 11.306 MOTA CA PRO A 356 2266 CB PRO A 356 23.539 12.301 18.604 1.00 28.11 MOTA 1.00 26.86 24.946 12.832 18.612 PRO A 356 ATOM 2267 CG 11.978 16.097 1.00 29.25 PRO A 356 23.363 55 MOTA 2268 C 12.537 1.00 27.27 2269 0 PRO A 356 24.304 15.529 ATOM 1.00 30.45 22.143 11.910 15.575 2270 N ALA A 357 ATOM 1.00 32.81 21.848 12.521 14.287 2271 CA ALA A 357 MOTA 20.507 12.019 13.757 1.00 31.99 MOTA 2272 CB ALA A 357

	ATOM	2273	C	ALA	Α	357		21.824	4	14.035	14.448	1.00 3	5.05	A
	ATOM	2274	0	ALA	Α	357		21.194		14.561	15.369	1.00 3	5.04	A
	ATOM	2275	N	LEU	A	358		22.516		14.730	13.552	1.00 3	7.81	A
	ATOM	2276	CA	LEU	Α	358		22.578	В	16.185	13.597	1.00 4	2.15	A
5	ATOM	2277	CB	LEU				23.679		16.681	12.658	1.00 3	9.54	A
	ATOM	2278	CG			358		25.086		16.285	13.109	1.00 3	9.51	A
	ATOM	2279		LEU				26.102		16.686	12.062	1.00 3	9.29	A
	ATOM	2280		LEU				25.395		16.953	14.445	1.00 4		A
	ATOM	2281	C			358		21.24		16.837	13.242	1.00 4		Α
10	MOTA	2282	o			358		20.874		16.927	12.069	1.00 4		A
10	ATOM	2283	N			359		20.53		17.290	14.275	1.00 5		A
	ATOM	2284	CA			359		19.223		17.939	14.140			A
	ATOM	2285	CB			359		19.353		19.428	13.726	1.00 5		A
	ATOM	2286		THR				19.999		19.521	12.448	1.00 5		A
15		2287		THR				20.158		20.204	14.763	1.00 5		A
15	MOTA		C			359		18.309		17.236	13.139	1.00 5		A
	MOTA	2288	0			359		18.483		16.016	12.930	1.00 5		A
	MOTA	2289		THR				17.40		17.908	12.595	1.00		A
	ATOM	2290			S					19.118	34.302	1.00		S
20	ATOM	2291	OH2		S	1 2		42.566		32.378	19.857	1.00		S
20	MOTA	2292	OH2					41.052			17.747	1.00		S
	ATOM	2293		TIP	S	3 5		37.014		33.030	18.152	1.00		s
	ATOM	2294		TIP	S	6		45.353		24.370 13.930	33.235	1.00 2		S
	MOTA	2295		TIP		7		31.896		22.781	28.249	1.00 2		S
25	MOTA	2296 2297		TIP		8		45.24		-0.589	-0.734	1.00		s
23	MOTA MOTA	2297		TIP	S	11		46.249		-0.348	-8.523	1.00 2		s
		2299		TIP		14		45.75		11.148	29.680	1.00 2		s
	MOTA MOTA	2300		TIP		15		44.27		13.157	34.592	1.00		S
	ATOM	2300				17		53.59		3.722	-1.720	1.00 2		S
30	ATOM	2301			s	18		46.04		13.087	31.565	1.00 2		s
30	ATOM	2302	OH2			19	•	53.42		22.401	-3.280	1.00 2		s
	ATOM	2304	OH2			20		34.58		7.922	5.383	1.00 2		s
	ATOM	2305		TIP		21		45.05		27.379	19.376	1.00 2		S
	ATOM	2305		TIP		23		28.89		36.416	28.633	1.00		S
35	ATOM	2307		TIP	s	24		35.53		11.645	-8.219	1.00 2		S
55	ATOM	2308		TIP		25		47.36		28.787	19.612	1.00 2		s
	ATOM	2309		TIP		27		48.85		21.588	12.634	1.00		S
	ATOM	2310		TIP	s	29		48.80		8.920	23.626	1.00 2		s
	ATOM	2311		TIP	_	31		48.61		7.247	10.112	1.00 2		S
40	ATOM	2312		TIP		34		44.82		28.720	15.621	1.00		S
	ATOM	2313		TIP	s	35		26.03		12.634	13.407	1.00	21.61	s
	ATOM	2314		TIP	S	36		50.46		19.810	40.066	1.00	25.45	s
	ATOM	2315		TIP	s	37		39.63		23.510	-0.239	1.00	30.88	s
	MOTA	2316		TIP		40		44.73		42.655	10.346	1.00	30.84	S
45	MOTA	2317		TIP		41		54.65		3.902	1.503	1.00	27.14	s
	MOTA	2318		TIP				45.69		21.923	39.754	1.00		S
	ATOM	2319		TIP				47.82		16.413	7.805	1.00	25.73	s
	ATOM	2320		TIP				50.29		31.412	29.642	1.00	32.79	s
	ATOM	2321		TIP				26.05	6	16.646	34.827	1.00	29.80	s
50	MOTA	2322		TIP				31.71	4	10.996	31.855	1.00	29.15	S
	ATOM	2323		TIP				46.10	8	23.843	-4.299	1.00	24.21	s
	ATOM	2324		TIP				37.64		11.206	34.448	1.00	28.56	s
	ATOM	2325		TIP				26.37		28.513	12.142	1.00	32.08	· S
	ATOM	2326		TIP				33.56		19.700	3.483	1.00	28.28	S
55	MOTA	2327		TIP				48.29		-0.632	14.280	1.00	32.13	S
-	ATOM	2328		TIP			•	40.06		26.036	34.324	1.00		S
	MOTA	2329		TIP				29.57	0	3.958	14.729	1.00		· S
	MOTA	2330		TIP				60.08	5	11.604	6.814	1.00		S
	ATOM	2331	OH2	TIP	S	73		39.20	3	44.403	18.686	1.00	26.61	s

	MOTA	2332	OH2	TIP	s	76	•	47.312	12.366	27.366	1.00 28.51	S
	MOTA	2333	OH2	TIP	s	80		43.862	33.771	33.329	1.00 28.82	S
	ATOM	2334	OH2	TIP	s	81		57.890	13.106	2.128	1.00 40.62	s
	ATOM	2335		TIP		82		41.663	34.381	32.043	1.00 19.35	s
5	ATOM	2336		TIP		85		50.974	40.331	19.200	1.00 21.14	. 8
_	ATOM	2337		TIP		88		47.925	-0.832	-6.556	1.00 24.11	s
	ATOM	2338		TIP		90		27.231	28.336	33.481	1.00 27.64	s
	ATOM	2339		TIP		91		43.651	-7.101	-7.995	1.00 24.33	s
	ATOM	2340		TIP		92		49.325	4.387	19.370	1.00 28.02	S
10	ATOM	2341		TIP	s	93		46.231	11.549	33.898	1.00 29.40	S
10	ATOM	2342		TIP		94		63.889	24.831	1.168	1.00 26.53	s
	MOTA	2343		TIP		96		56.396	4.952	-6.749	1.00 28.00	s
	ATOM	2344		TIP		98		35.510	27.986	11.558	1.00 29.24	s
	ATOM	2345		TIP				49.942	24.366	30.265	1.00 31.61	s
15	MOTA	2346		TIP				56.121	7.113	-8.298	1.00 31.57	s
13		2347		TIP		102		58.318	19.957	-8.378	1.00 26.95	s
	ATOM ATOM	2347	OH2	TIP				49.647	22.446	39.624	1.00 40.57	s
				TIP				45.359	7.052	13.052	1.00 26.27	S
	ATOM	2349		TIP		104		37.150	32.340	32.346	1.00 20.27	S
20	ATOM	2350		TIP				43.465	40.457	8.240	1.00 40.48	S
20	MOTA	2351		TIP					8.257	13.418	1.00 30.70	S
	MOTA	2352						36.644 41.912	-8.974	-8.264	1.00 26.08	S
	MOTA	2353	OH2			123			15.800	-7.411	1.00 24.08	S
	MOTA	2354	OH2					62.424 37.266			1.00 24.00	S
25	MOTA	2355	OH2					43.129	18.656 26.845	14.606	1.00 25.19	s
25	MOTA	2356 2357		TIP		127		36.339	32.639	29.802	1.00 29.25	s
	ATOM	2357	OH2 OH2			130		54.051	14.561	26.498	1.00 23.23	s
•	ATOM	2359		TIP		131		41.805	-4.242	5.492	1.00 33.72	· s
	ATOM ATOM	2359	OH2					38.873	25.163	36.697	1.00 30.69	s
30		2360	OH2					28.777	8.553	25.307	1.00 31.43	S
30	ATOM	2362		TIP		135		53.672		-12.803	1.00 33.45	s
	ATOM ATOM	2362		TIP				59.892	15.434	11.467	1.00 31.39	s
	ATOM	2364		TIP				31.040	12.361	35.470	1.00 34.07	s
	ATOM	2365		TIP		139		33.489	14.292	-0.598	1.00 40.68	S
35	ATOM	2366		TIP				46.918	8.748	11.662	1.00 29.23	s
55	ATOM	2367		TIP				46.297	-7.287	-9.196	1.00 42.20	S
	ATOM	2368		TIP		142		58.193	6.715	-4.685	1.00 35.48	S.
	ATOM	2369		TIP				44.598	4.435	12.503	1.00 27.68	S
	ATOM	2370		TIP				27.003	5.999	12.450	1.00 36.30	S
40	ATOM	2371		TIP		145		43.676	32.852	35.735	1.00 35.70	S
-10	ATOM	2372		TIP				35.783	18.628	36.452	1.00 34.62	s
	ATOM	2372		TIP				25.402	4.058	20.638	1.00 45.03	s
	ATOM	2374		TIP		148		45.839	35.853	33.724	1.00 35.47	s
	ATOM	2375		TIP				22.176	18.976	16.752	1.00 31.87	s
45	MOTA	2376		TIP	_			43.986	33.179		1.00 37.70	S
	ATOM	2377		TIP				50.653		42.428	1.00 35.80	S
	ATOM	2378		TIP				47.843		9.506	1.00 31.05	s
	ATOM	2379		TIP				44.693		-14.175	1.00 29.90	· S
	ATOM	2380		TIP				26.560	36.851	31.684	1.00 49.29	s
50	ATOM	2381		TIP				46.867		-12.951	1.00 29.21	s
50	ATOM	2382		TIP				30.432		12.438	1.00 37.76	· s
	ATOM	2383		TIP				41.004		6.423	1.00 39.53	s
	ATOM	2384		TIP				49.258			1.00 33.97	s
	ATOM	2385		TIP				48.082			1.00 33.10	s
55	ATOM	2386		TIP				47.448			1.00 34.87	s
	MOTA	2387		TIP				19.687		23.411	1.00 35.01	S
	MOTA	2388		TIP				32.402			1.00 37.26	s
	ATOM	2389		TIP				39.475		33.237	1.00 35.34	S
	ATOM	2390		TIP				44.277	18.950	5.162	1.00 45.14	S

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	ATOM	2391	OH2 TIP S 166	34.797	30.523	10.736	1.00 47.55	S
	MOTA	2392	OH2 TIP S 167	46.541		-14.949	1.00 26.54	S
	MOTA	2393	OH2 TIP S 168	36.333	16.371	1.539	1.00 38.68	S
	ATOM	2394	OH2 TIP S 169	46.761	38.936	27.403	1.00 34.66	s
5	ATOM	2395	OH2 TIP S 170	24.163	13.264	11.375	1.00 41.23	S
	ATOM	2396	OH2 TIP S 171	48.459	15.018	31.951	1.00 38.11	S
	MOTA	2397	OH2 TIP S 172	34.261	23.193	40.004	1.00 48.96	s
	MOTA	2398	OH2 TIP S 173	45.924	-0.026	13.224	1.00 39.55	s s
	MOTA	2399	OH2 TIP S 175	41.384	37.389	32.543	1.00 40.74	
10	ATOM	2400	OH2 TIP S 177	49.394	35.312	27.150	1.00 44.33	s s
	ATOM	2401	OH2 TIP S. 178	29.066	29.942	34.359	1.00 41.46	S
	MOTA	2402	OH2 TIP S 180	49.354	19.467	7.273	1.00 34.56 1.00 47.74	S
	MOTA	2403	OH2 TIP S 181	25.298	17.029	31.863	1.00 47.74	S
	MOTA	2404	OH2 TIP S 182	37.071	25.027	4.669	1.00 43.87	S
15	MOTA	2405	OH2 TIP S 183	22.581	7.487	18.691	1.00 41.75	S
	ATOM	2406	OH2 TIP S 184	32.269	7.011	-1.891	1.00 48.84	s
	MOTA	2407	OH2 TIP S 185	48.234	0.494	6.833	1.00 45.27	s
	ATOM	2408	OH2 TIP S 187	20.008	14.658	19.211	1.00 43.27	s
	MOTA	2409	OH2 TIP S 188	49.341	22.698	42.272 -8.097	1.00 42.20	s
20	MOTA	2410	OH2 TIP S 190	61.292	18.260	2.819	1.00 40.38	s
	MOTA	2411	OH2 TIP S 191	28.152	10.606 12.619	23.191	1.00 34.27	s
*•	MOTA	2412	OH2 TIP S 192	25.626	11.603	1.216	1.00 46.54	S
	MOTA	2413	OH2 TIP S 193	59.876		-10.646	1.00 45.82	s
	MOTA	2414	OH2 TIP S 194	57.592	36.649	21.499	1.00 38.73	S
25	MOTA	2415	OH2 TIP S 195	31.509	-1.543	-6.136	1.00 42.66	S
	MOTA	2416	OH2 TIP S 197		8.729	13.088	1.00 42.78	S
	ATOM	2417	OH2 TIP S 198	24.467 38.098	8.699	25.759	1.00 32.80	S
	MOTA	2418	OH2 TIP S 199 OH2 TIP S 200	57.831		-13.255	1.00 45.31	S
	ATOM	2419	OH2 TIP S 200 OH2 TIP S 201	23.888	22.328	30.524	1.00 37.12	S
30	MOTA	2420	OH2 TIP S 201	47.691	26.068	37.666	1.00 37.92	S
	MOTA	2421	OH2 TIP S 202	38.653	7.070	29.307	1.00 50.54	S
	MOTA	2422 2423	OH2 TIP S 206	44.424	27.583	2.092	1.00 53.50	S
	. ATOM	2423	OH2 TIP S 212	22.258	2.296	17.948	1.00 47.38	S
35	MOTA MOTA	2425	OH2 TIP S 214	19.843	17.943	23.303	1.00 30.36	S
33	MOTA	2425	OH2 TIP S 216	27.647	11.344	24.681	1.00 31.32	S
	ATOM	2427	OH2 TIP S 217	37.953	7.817	-9.284	1.00 45.97	S -
	ATOM	2428	OH2 TIP S 218	33.845	34.040	12.124	1.00 38.11	S
	ATOM	2429	OH2 TIP S 219	58.484	15.269	13.717	1.00 38.26	S
40	ATOM	2430	OH2 TIP S 220	48.526	40.920	26.583	1.00 35.23	S
40	MOTA	2431	OH2 TIP S 222	52.094	21.184	38.122	1.00 29.86	S
	ATOM	2432	OH2 TIP S 223	36.889			1.00 37.63	S
	MOTA	2433	OH2 TIP S 224	47.642	-1.401	-10.684	1.00 34.89	S
	MOTA	2434	OH2 TIP S 226	47.284	2.916		1.00 34.10	S
45	MOTA	2435	OH2 TIP S 227	42.468		-15.039	1.00 37.98	S
,	MOTA	2436	OH2 TIP S 228	19.169			1.00 41.57	
	ATOM	2437	OH2 TIP S 231	57.592			1.00 50.22	S
	MOTA	2438	OH2 TIP S 232	27.102			1.00 40.57	S
	ATOM	2439	OH2 TIP S 233	58.618			1.00 50.71	S
50	ATOM	2440		22.822			1.00 34.93	S · S
	MOTA	2441	OH2 TIP S 236	24.831			1.00 37.69	S
	MOTA	2442		20.045			1.00 39.57	S. S
	MOTA	2443		58.019			1.00 41.42	S
	MOTA	2444		19.490			1.00 34.55 1.00 39.68	S
55	ATOM	2445		61.187				S
	MOTA	2446		33.680				s
	MOTA	2447		51.539				s
	MOTA	2448		25.872				s
	MOTA	2449	OH2 TIP S 248	37.332	5.849	9.544	T.00 43.01	

	ATOM	2450	OH2 TIP S 250	39.087	-1.293	-9.655	1.00 42.96	S
	ATOM	2451	OH2 TIP S 258	23.938	30.000	30.010	1.00 38.89	S
	ATOM	2452	OH2 TIP S 259	24.949	29.749	32.578	1.00 40.17	S
	ATOM	2453	OH2 TIP S 260	32.111	17.986	1.918	1.00 48.36	S
5	ATOM	2454	OH2 TIP S 266	21.404	12.876	25.603	1.00 57.17	S
•	ATOM	2455	OH2 TIP S 269	35.425	36.767	12.550	1.00 30.70	S
	ATOM	2456	OH2 TIP S 270	52.438	25.529	30.131	1.00 44.85	S
	ATOM	2457	OH2 TIP S 271	53.299	20.156	36.003	1.00 37.15	S
	MOTA	2458	OH2 TIP S 272	50.914	6.919	23.723	1.00 43.29	S
10	ATOM	2459	OH2 TIP S 274	31.578	30.795	11.014	1.00 50.15	S
10		2450	OH2 TIP S 275	26.341	7.243	22.447	1.00 39.40	S
	ATOM	2460	OH2 TIP S 276	60.392	18.195	10.235	1.00 37.91	S
	MOTA		OH2 TIP S 277	47.355	-9.081		1.00 48.18	S
	ATOM	2462	OH2 TIP S 277	41.304		-16.647	1.00 38.12	S
	MOTA	2463	OH2 TIP S 275	33.299	21.620	37.881	1.00 46.29	S
15	ATOM	2464	OH2 TIP S 283	56.469	26.112	-8.575	1.00 43.71	S
	ATOM	2465	OH2 TIP S 283	48.382	26.573	7.246	1.00 41.43	s
	ATOM	2466	OH2 TIP S 288	56.240		-11.331	1.00 41.79	S
	MOTA	2467		49.060	14.978	28.166	1.00 37.03	s
	ATOM	2468	OH2 TIP S 290		44.270	26.442	1.00 45.08	S
20	MOTA	2469	OH2 TIP S 291	37.095	-0.384		1.00 48.60	S
	ATOM	2470	OH2 TIP S 292	47.814	2.784	-7.841	1.00 41.89	S
	MOTA	2471	OH2 TIP S 297	58.081	•	18.644	1.00 54.91	S
	MOTA	2472	OH2 TIP S 298	36.447	45.321	1.767	1.00 30.55	S
	MOTA	2473	OH2 TIP 5 299	49.029	23.328	8.634	1.00 48.47	S
25	MOTA	2474	OH2 TIP S 301	24.375	13.771		1.00 35.76	S
	MOTA	2475	OH2 TIP S 303	47.904	36.798	28.653 27.172	1.00 43.59	S
	MOTA	2476	OH2 TIP S 305	51.156	40.821	35.227	1.00 42.60	S
	MOTA	2477	OH2 TIP S 306	32.943	28.917	6.251	1.00 46.15	s
	MOTA	2478	OH2 TIP S 307	58.462	28.373	36.712	1.00 48.26	S
30	MOTA	2479	OH2 TIP S 308	41.964	30.940	-3.336	1.00 50.61	S
	MOTA	2480	OH2 TIP S 313	51.176	-1.922	23.805	1.00 36.97	S
	ATOM	2481	OH2 TIP S1001	21.319	36.868	27.617	1.00 44.40	S
	MOTA	2482 •		48.880	32.620	11.767	1.00 45.49	- S
	ATOM	2483	OH2 TIP S1003	61.880	19.473	26.815	1.00 24.43	S
35	ATOM	2484	OH2 TIP S1004	52.770	21.424	36.197	1.00 35.97	S
	MOTA	2485	OH2 TIP S1005	35.373	29.094	4.389	1.00 33.37	S
	MOTA	2486	OH2 TIP S1006	40.815	-6.636	11.272	1.00 49.45	s
	ATOM	2487	OH2 TIP S1007	44.953	1.286	27.009	1.00 48.51	S
	ATOM	2488	OH2 TIP S1010	21.004	16.168		1.00 50.10	S
40	MOTA	2489	OH2 TIP S1011	47.094	41.786	9.243	1.00 30.10	S
	MOTA	2490	OH2 TIP S1012	32.479	2.978	14.158	1.00 40.72	G
•	MOTA	2491	012 GLC G 1	48.557		-12.279	1.00 38.05	G
	MOTA	2492	C11 GLC G 1	48.836		-11.097	1.00 38.09	G
	MOTA	2493	C13 GLC G 1	49.266		-11.476	1.00 33.99	G
45	MOTA	2494	O14 GLC G 1	49.559		-10.292	1.00 37.32	G
	ATOM	2495	C15 GLC G 1	48.150		-12.257	1.00 37.32	G
	MOTA	2496	O16 GLC G 1	48.574		-12.604	1:00 33.74	G
	MOTA	2497	O12 GLC G 2	40.114	-6.634	-6.562	1.00 33.32	G
	MOTA	2498	C11 GLC G 2	38.967	-6.592	-7.404	1.00 31.05	G
50	MOTA	2499	C13 GLC G 2	37.712	-6.417	-6.552	1.00 31.30	G
	ATOM	2500	O14 GLC G 2	36.554	~6.406	-7.389		G
	MOTA	2501	C15 GLC G 2	37.792	-5.109	-5.761	1.00 30.03 1.00 29.66	G
	ATOM	2502	O16 GLC G 2	36.609	-4.961	-4.975		G
	MOTA	2503	O12 GLC G 3	44.030		-13.470		G
55	MOTA	2504	C11 GLC G 3	43.950		-13.690		G
	MOTA	2505	C13 GLC G 3	42.747		-14.579		
	ATOM	2506	O14 GLC G 3	41.551		-13.942		G
	MOTA	2507		42.878		-15.934		G
	MOTA	2508		41.736	9.613	-16.731	1.00 40.78	G

	MOTA	2509	012	GLC	G	5		40.556	1.005	2.289	1.00 45.25	G
	ATOM	2510	C11	GLC	G	5		40.966	2.332	1.960	1.00 40.56	G
	ATOM	2511	C13	GLC	G	5		40.187	3.327	2.814	1.00 40.36	G
	ATOM	2512	014	GLC	G	5		38.791	3.169	2.572	1.00 40.71	G
5	ATOM	2513	C15	GLC	G	5		40.619	4.751	2.464	1.00 40.04	G
-	ATOM	2514		GLC		5		39.885	5.681	3.256	1.00 36.89	G
	ATOM	2515		GLC		6		36.951	22.702	40.046	1.00 63.04	G
	ATOM	2516		GLC		6		37.592	21.583	39.422	1.00 62.46	G
	MOTA	2517		GLC		6		38.104	21.978	38.030	1.00 61.14	G
10	ATOM	2518		GLC		6		39.034	23.054	38.168	1.00 61.72	G
10		2518		GLC		6		36.948	22.429	37.126	1.00 60.51	G
	ATOM	2520		GLC		6		35.992	21.372	36.960	1.00 58.61	G
	ATOM			GLC		. 7		37.316	0.281	14.299	1.00 73.45	· G
	MOTA	2521		GLC							1.00 73.43	G
15	ATOM	2522				7		37.655	-0.758	15.222		G
15	ATOM	2523		GLC		7		36.592	-1.856	15.157	1.00 72.98	
	MOTA	2524		GLC		7		35.320	-1.299	15.498	1.00 73.88	G
	MOTA	2525		GLC		7		36.924	-2.989	16.134	1.00 73.66	G
	MOTA	2526		GLC		7		36.972	-2.493	17.478	1.00 75.38	G,
_	MOTA	2527		GLC		8		51.921	21.898	5.908	1.00 62.51	G
20	MOTA	2528	-	GLC		8		52.447	20.871	5.063	1.00 63.42	. G
	ATOM	2529		GLC		8		51.476	20.597	3.908	1.00 64.28	G
	MOTA	2530		${\tt GLC}$		8	•	51.297	21.794	3.150	1.00 66.28	G
	ATOM	2531	C15	GLC	G	8		50.121	20.137	4.448	1.00 64.49	G
	MOTA	2532		GLC		8		49.233	19.886	3.357	1.00 64.01	G
25	ATOM	2533	012	GLC	G	10		36.044	37.499	29.523	1.00 56.89	G
	ATOM	2534	C11	GLC	G	10		35.164	36.645	30.259	1.00 56.97	G
	MOTA	2535	C13	GLC	G	10		33.849	36.489	29.494	1.00 56.11	G
	MOTA	2536	014	GLC	G	10		33.248	37.772	29.308	1.00 56.44	G
	ATOM	2537	C15	GLC	G	10		32.900	35.580	30.277	1.00 55.84	G
30	MOTA	2538	016	GLC	G	10		31.674	35.442	29.557	1.00 55.39	G
	ATOM	2539	03G	ATP	N	1		46.280	25.658	5.170	1.00 51.49	N
	ATOM	2540	PG	ATP	N	1		46.464	25.053	3.691	1.00 52.22	N
	ATOM	2541	01G	ATP	N	. 1		47.406	23.911	3.763	1.00 51.41	N
	ATOM	2542	02G	ATP	N	1		46.794	26.182	2.784	1.00 52.07	N
35	ATOM	2543	03B	ATP	N	1		44.976	24.513	3.344	1.00 51.01	N
	ATOM	2544	PB	ATP		1		44.560	22.969	3.605	1.00 50.20	N
	MOTA	2545	01B	ATP	N	1		43.083	22.898	3.669	1.00 49.41	N
	ATOM	2546		ATP		1		45.345	22.474	4.766	1.00 50.34	N
	MOTA	2547		ATP		1		45.070	22.231	2.255	1.00 47.77	N
40	ATOM	2548	PA	ATP		1		45.075	20.613	2.121	1.00 42.84	N
	ATOM	2549		ATP		1.		45.547	20.291	0.754	1.00 43.81	N
	ATOM	2550		ATP		1		45.807	20.035	3.270	1.00 45.03	N
	ATOM	2551		ATP		ī		43.516	20.223	2.245	1.00 41.73	N
	ATOM	2552		ATP		1		42.528	20.925	1.489	1.00 37.57	N
45	ATOM	2553		ATP		1		41.127			1.00 39.45	N
73	ATOM	2554		ATP		1		40.907	19.024	1.279	1.00 37.72	Ŋ
	MOTA	2555		ATP		1		40.777	20.321	3.251	1.00 38.48	N
	ATOM	2556		ATP		ı		40.360	21.615	3.697	1.00 40.42	N
				ATP		1		39.608	19.374	3.270	1.00 37.58	N
50	ATOM	2557				1			20.076	2.924	1.00 37.30	N
50	ATOM	2558		ATP				38.410		2.173	1.00 35.55	N
	ATOM	2559		ATP		1		39.939	18.346	2.747	1.00 33.35	N
	ATOM	2560	И9	ATP		1		40.628	17.156	3.274	1.00 31.78	N
	MOTA	2561	C8	ATP		1		41.864	17.126	3.274	1.00 30.49	N
·	ATOM	2562	N7	ATP		1		42.143	15.877			N
55	ATOM	2563	C5	ATP		1		41.088	15.118	3.390	1.00 27.49	N
	ATOM	2564	C4	ATP		1		40.125	15.925	2.810	1.00 30.02	N
	MOTA	2565	N3	ATP		1		38.937	15.389	2.431	1.00 27.11	
	ATOM	2566	C2	ATP		1		38.679	14.085	2.615	1.00 25.62	N
	ATOM	2567	Nl	ATP	N	1		39.597	13.283	3.175	1.00 21.76	Ŋ

											**
	MOTA	2568	C6	ATP :	N	1	40.800	13.768	3.571	1.00 23.90	N
	MOTA	2569	Иб	ATP :	N	1	41.698	12.964	4.127	1.00 21.94	N
	ATOM	2570	S	S04	I	1 .	58.680	8.493	-0.639	1.00 56.05	I
	MOTA	2571	01	504	I	1	57.956	7.875	0.483	1.00 58.83	I
5	MOTA	2572	02	SO4	I	1	57.886	9.607	-1.188	1.00 57.04	I
	ATOM	2573	03	SO4	I	1	58.906	7.478	-1.683	1.00 57.47	I
	ATOM	2574	04	SO4	I	1	59.976	9.008	-0.156	1.00 57.51	I
	ATOM	2575	s	SO4	I	2	39.339	4.855	7.057	1.00 84.24	ĭ
	ATOM	2576	01	SO4	I	2	39.390	6.175	7.711	1.00 85.02	I
10	ATOM	2577	02	SO4	I	2 ်	40.101	4.897	5.797	1.00 84.75	I
	MOTA	2578	03	SO4	I	2	37.936	4.506	6.766	1.00 84.94	I
	MOTA	2579	04	SO4	I	2	39.931	3.842	7.954	1.00 84.44	I
	ATOM	2580	s	SO4	I	3	38.987	-2.256	3.310	1.00 58.58	I
	MOTA	2581	01	SO4	I	3	37.734	-1.675	3.827	1.00 59.11	I
15	MOTA	2582	02	S04	I	3	39.460	-1.454	2.172	1.00 59.91	I
••	ATOM	2583	03	SO4	I	3	38.743	-3.640	2.866	1.00 60.97	I
	ATOM	2584	04	SO4	I	3	40.014	-2.260	4.369	1.00 59.58	I
	MOTA	2585	s	SO4	I	4	34.397	5.289	30.981	1.00 64.34	I
	MOTA	2586	01	SO4	I	4	33.627	6.528	30.742	1.00 60.43	I
20	ATOM	2587	02	SO4	I	4	34.337	4.427	29.782	1.00 60.11	I
	ATOM	2588	03	SO4	I	4	33.816	4.572	32.133	1.00 64.39	I
	ATOM	2589	04	SO4	I	4	35.806	5.626	31.277	1.00 63.55	. I
	ATOM	2590	s	SO4	I	5	55.074	-6.984	-3.711	1.00 75.40	I
	MOTA	2591	01	SO4	I	5	54.657	-7.518	-2.399	1.00 74.66	ī
25	MOTA	2592	02	SO4	I	5	54.209	-5.845	-4.065	1.00 74.96	. I
	ATOM	2593	03	SO4	I	5	54.950	-8.034	-4.742	1.00 74.22	I
	ATOM	2594	04	SO4	I	5	56.477	-6.532	-3.633	1.00 75.15	I
	ATOM	2595	02	PO4	P	100	57.362	24.998	13.149	1.00 66.76	P
	ATOM	2596	03	PO4	P	100	59.399	26.166	13.761	1.00 66.89	P
30	ATOM	2597	04	PO4	P	100	57.761	25.606	15.462	1.00 67.43	P
20	ATOM	2598	01	PO4	P	100	57.264	27.325	13.818	1.00 65.91	P
	ATOM	2599	P	PO4	P	100	57.947	26.025	14.048	1.00 66.69	P
	END						,				

Example 4: Co-ordinates for the dimer of the PDK1 fragment, without alternate side chains. Chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

			CD.	PRO A	71	58.912	-7.251	8.216	1.00 6	7.78	A
	MOTA	1	CB		. –	• • • •	-6.941	9.534	1.00 6	9.16	A
. 40	ATOM	2	CG	PRO A	71	59.621			1.00 6		A
	ATOM	3	C	PRO A	71	59.493	-6.506	5.894			A
	ATOM	4	0	PRO A	71	59.196	-5.318	5.766	1.00 6		
	ATOM	5	N	PRO A	71	60.984	-6.073	7.833	1.00 €	7.86	A
	MOTA	6	CD	PRO A	71	60.554	-5.762	9.207	1.00 6	8.24	A
A E	ATOM	7	CA	PRO A	71	60.040	-7.035	7.217	1.00 €	7.75	, A
45		•		PRO A	72	59.356	-7.385	4.890	1.00 6	6.32	. A
	MOTA	8	N ·				-8.816	4.898	1.00 6		A
	MOTA	9	CD	PRO A	72	59.712	_		1.00 6		A
	MOTA	10	CA	PRO A	72	58.840	-6.986	3.578			A
	MOTA	11	CB	PRO A	72	58.672	-8.321	2.858	1.00		
50	ATOM	12	CG	PRO A	72	59.796	-9.133	3.419	1.00 6		A
50	ATOM	13	C	PRO A	72	57.527	-6.208	3.673	1.00 6	53.94	A
			-	PRO A		56.710	-6.451	4.561	1.00	54.11	Α
	MOTA	14	0			= -	-5.268	2.753	1.00		A
	MOTA	15	N	ALA A		57.341	- ·		1.00		A
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708			A
55	MOTA	17	CB	ALA A	73	56.438	-3.030	3.165	1.00	58.05	. A

										_
	ATOM	18	C	ALA A	73	55.626	-4.448	1.271	1.00 56.78	A.
	ATOM	19	0	ALA A	73	56.347		0.349	1.00 56.95	A
	ATOM	20	N	PRO A	74	54.372	-4.024	1.057	1.00 54.15	A
	ATOM	21	CD	PRO A	74	53.335	-3.610	2.018	1.00 53.31	A
5	ATOM	22	CA	PRO A	74	53.856	-4.003	-0.314	1.00 52.54	Α.
_	ATOM	23	CB	PRO A	74	52.474	-3.375	-0.148	1.00 52.86	A
	ATOM	24	CG	PRO A	74	52.067	-3.824	1.226	1.00 52.88	A
	ATOM	25	C	PRO A	74	54.772	-3.167	-1.204	1.00 50.08	A
	ATOM	26	ō	PRO A	74	55.559	-2.361	-0.708	1.00 49.96	A
10		27	N	ALA A	75	54.680	-3.366	-2.514	1.00 47.58	A
10	MOTA			ALA A	75	55.503	-2.602	-3.446	1.00 44.69	A
	ATOM	28	CA			55.312	-3.121	-4.870	1.00 46.14	A
	MOTA	29	CB	ALA A	75	55.100	-1.134	-3.371	1.00 41.55	A
	MOTA	30	C	ALA A	75			-3.086	1.00 41.01	A
	MOTA	31	0	ALA A	75	53.947	-0.813		1.00 38.31	A
15	MOTA	32	И	LYS A	76	56.053	-0.245	-3.619		A
	ATOM	33	CA	LYS A	76	55.781	1.184	-3.588	1.00 35.72	
	MOTA	34	CB	LYS A	76	57.053	1.957	-3.930	1.00 37.70	A
	MOTA	35	CG	LYS A	76	57.123	3.356	-3.350	1.00 40.99	A
	ATOM	36	CD	LYS A	76	57.262	3.316	-1.836	1.00 40.04	A
20	ATOM	37	CE	LYS A	76	57.511	4.705	-1.277	1.00 42.08	A
	ATOM	38	NZ	LYS A	76	57.681	4.695	0.202	1.00 42.99	A
	ATOM	39	C	LYS A	76	54.708	1.467	-4.638	1.00 32.65	A
	ATOM	40	ŏ	LYS A	76	54.814	1.005	-5.770	1.00 31.41	A
	ATOM	41	N	LYS A	77	53.668	2.207	-4.270	1.00 28.59	A
25		42	CA	LYS A	77	52.619	2.517	-5.232	1.00 25.72	A
25	ATOM			LYS A	77	51.316	2.865	-4.509	1.00 26.22	A
	MOTA	43	CB		77	50.796	1.731	-3.631	1.00 27.15	A
	MOTA	44	CG	LYS A		49.487	2.089		1.00 26.80	A
	MOTA	45	CD	LYS A	77	49.487	1.091	-1.870	1.00 27.31	A
	MOTA	46	CE	LYS A	77		-0.296	-2.380	1.00 27.17	A
30	MOTA	47	NZ	LYS A	77	48.998		-6.137	1.00 27.17	A
	MOTA	48		LYS A	77	53.053	3.668		1.00 21.60	A
	MOTA	49	0	LYS A	77	54.010	4.377	-5.829	1.00 21.00	A
	MOTA	50	N	ARG A	78	52.351	3.838	-7.254		A
	MOTA	51	CA	ARG A	78	52.662	4.897	-8.211	1.00 26.14	
35	MOTA	52	CB	ARG A	78	53.574	4.344	-9.318	1.00 28.57	A
	ATOM	53	CG	ARG A	78	53.017		-10.050	1.00 34.78	A
	ATOM	54	CD	ARG A	78	54.092		-10.896	1.00 40.96	A
	ATOM	55	NE	ARG A	78	53.560	1.364	-11.700	1.00 48.93	A
	ATOM	56	CZ	ARG A		52.985	0.270	-11.203	1.00 52.58	Α
40	ATOM	57		ARG A		52.860	0.113	-9.889	1.00 54.60	A
40	ATOM	58		ARG A		52.530	-0.672	-12.022	1.00 54.09	A
		59	C	ARG A		51.382	5.488	-8.803	1.00 23.76	A
	MOTA	60	0	ARG A		50.311	4.888	-8.706	1.00 24.25	A
	MOTA		N	PRO A		51.475	6.676	-9.428	1.00 21.76	A
4.5	ATOM	61		PRO A		52.691	7.475	-9.668	1.00 20.82	A
45	ATOM	62	CD			50.301		-10.021	1.00 21.96	Α
	ATOM	63	CA	PRO A		50.910		-10.816	1.00 22.27	A
	MOTA	64	CB	PRO A				-10.014	1.00 22.12	A
	MOTA	65	CG	PRO A		52.124		-10.903	1.00 22.86	A
	MOTA	66	С	PRO A		49.446			1.00 20.52	A
50	ATOM	67	0	PRO A		48.213		-10.842	1.00 20.32	A
	ATOM	68	N	GLU A		50.103		-11.714		A
	MOTA	69	CA	GLU A	80	49.403		-12.628		
	MOTA	70	CB	GLU A	80	50.393		-13.571		A N
	MOTA	71	CG	GLU A	80	51.230		-12.925		A
55	ATOM	72		GLU A	80	52.157		-13.913		A
	ATOM	73		1 GLU A	80	53.072		-14.433		A
	ATOM	74		2 GLU P		51.969		-14.172		A
	MOTA	75		GLU A		48.556	3.631	-11.912	1.00 22.09	A
	MOTA	76		GLU A		47.692		-12.530	1.00 22.37	A
	ATOM	, 0								

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	MOTA	77	Ŋ	ASP .		81		.48.804		-10.622	1.00 19.97	A
	ATOM	78	CA	ASP		81		48.026	2.423	-9.874	1.00 19.93	A
	MOTA	79	CB	ASP		81		48.736	2.029	-8.571	1.00 21.19	A
	MOTA	80	CG	ASP		81		50.089	1.380	-8.807	1.00 22.46	A
5	ATOM	81		ASP		81		50.195	0.554	-9.731	1.00 24.22	A
	MOTA	82	OD2	ASP		81		51.043	1.685	-8.058	1.00 23.33	A
	ATOM	83	С	ASP		81		46.652	2.975	-9.518	1.00 20.85	A
	ATOM	84	0	ASP		81		45.793	2.246	-9.015	1.00 19.96	A
	ATOM	85	N	PHE		82		46.445	4.258	-9.804	1.00 18.91	A
10	ATOM	86	CA	PHE		82		45.200	4.934	-9.465	1.00 19.30	A
	MOTA	87	CB	PHE		82		45.475	6.027	-8.427	1.00 18.43	A
•	MOTA	88	CG	PHE	Α	82		46.134	5.531	-7.175	1.00 18.01	A
	MOTA	89	CD1	PHE	A	82		45.371	5.136	-6.084	1.00 17.19	A
	ATOM	90		PHE		82		47.520	5.460	-7.086	1.00 18.99	A
15	MOTA	91		PHE	Α	82		45.977	4.676	-4.918	1.00 17.12	A
	MOTA	92	CE2	PHE	Α	82 ~		48.137	5.000	-5.925	1.00 19.64	A
	MOTA	93	CŹ	PHE		82		47.361	4.607	-4.838	1.00 18.00	A
	MOTA	94	С	PHE	Α	82		44.476		-10.621	1.00 20.81	A
	ATOM	95	0	PHE	Α	82		45.066		-11.649	1.00 20.34	A
20	ATOM	96	N	LYS	Α	83		43.182		-10.411	1.00 19.80	A
	MOTA	97	CA	LYS	Α	83		42.321		-11.353	1.00 21.65	A
	MOTA	98	CB	LYS	Α	83		41.096	5.625	-11.687	1.00 22.02	Α
	MOTA	99	CG	LYS	A	83		40.062		-12.550	1.00 28.93	A
	ATOM	100	CD	LYS	Α	83		38.974	5.355	-12.981	1.00 34.20	A
25	MOTA	101	CE	LYS	Α	83		37.909		-13.824	1.00 38.10	A
	MOTA	102	NZ	LYS	Α	83		37.179	7.086	-13.043	1.00 43.33	, A
	ATOM	103	C	LYS	Α	83		41.913		-10.541	1.00 20.74	A
	MOTA	104	0	LYS	Α	83		41.084	7.606	-9.635	1.00 20.98	A
	MOTA	105	N	PHE	Α	84		42.513		-10.835	1.00 19.99	A
30	ATOM	106	CA	PHE	Α	84		42.188	10.049	-10.083	1.00 18.63	A
	ATOM	107	CB	PHE	Α	84		43.279	11.103	-10.258	1.00 18.95	A
	MOTA	108	CG	PHE	Α	84		44.571	10.741	-9.587	1.00 17.68	A
	ATOM	109	CD1	PHE	A	84		45.498		-10.224	1.00 18.16	A
	ATOM	110	CD2	PHE	Α	84		44.843	11.183	-8.299	1.00 19.66	A
35	ATOM	111	CE1	PHE	Α	84		46.676	9.556	-9.589	1.00 18.09	Α
	ATOM	112	CE2	PHE	Α	84		46.021	10.816	-7.653	1.00 18.89	A
	ATOM	113	cz	PHE	Α	84		46.936	10.002	-8.301	1.00 17.33	A
	ATOM	114	C	PHE	Α	84		40.834	10.617	-10.460	1.00 19.69	A
	ATOM	115	0	PHE	A	84	•	40.391	10.489	-11.601	1.00 20.72	A
40	ATOM	116	N	GLY	Α	85		40.178	11.233	-9.484	1.00 16.80	A
	ATOM	117	CA	GLY	Α	85		38.872	11.810	-9.716	1.00 17.73	A
	ATOM	118	С	GLY	Α	85		38.819	13.280	-9.346	1.00 18.75	A
	ATOM	119	0	GLY	Α	85		39.740	14.043	-9.650°	1.00 18.45	A
	ATOM	120	N	LYS	Α	86		37.753	13.673	-8.659	1.00 16.00	A
45	ATOM	121	CA	LYS	Α	86		37.571	15.064	-8.278	1.00 18.26	A
	MOTA	122	CB	LYS		86		36.133	15.302	-7.812	1.00 19.00	A
	MOTA	123	CG	LYS	A	86		35.793	14.660	-6.481	1.00 21.55	A
	MOTA	124	CD	LYS		86		34.368	14.981	-6.066	1.00 26.48	A
	ATOM	125	CE	LYS		86		33.994	14.239		1.00 31.92	A
50	ATOM	126	NZ.			86		32.568	14.457	-4.412	1.00 35.36	A
-	ATOM	127	C	LYS		86		38.523	15.571	-7.202	1.00 18.57	A
	ATOM	128	0	LYS		86		39.045	14.807	-6.385	1.00 16.77	Α
	ATOM	129	N	ILE		87		38.737	16.881	-7.227	1.00 17.88	A
	ATOM	130	CA	ILE				39.577	17.554	-6.256	1.00 18.26	A
55	ATOM	131	СВ	ILE		87		39.994	18.952	-6.772	1.00 19.60	A
	MOTA	132		ILE		87		40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133		ILE		87		40.968	18.786	-7.945	1.00 21.16	A
	ATOM	134		ILE		87		41.412	20.087	-8.588	1.00 25.26	A
	ATOM	135	С	ILE		87		38.731	17.709	-4.997	1.00 19.67	A

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	MOTA	136	0	ILE	Α	87	37.628	18.249	-5.052	1.00 20.41	Α
	MOTA	137	N	LEU	A	88	39.240	17.229	-3.867	1.00 19.15	A
	MOTA	138	CA	LEU	A	88	38.508	17.324	-2.611	1.00 20.68	Α
	MOTA	139	CB	LEU	Α	88	38.870	16.151	-1.700	1.00 19.97	A
5	ATOM	140	CG	LEU	Α	88	38.529	14.759	-2.237	1.00 19.24	A
	MOTA	141	CD1	LEU	A	88	39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142	CD2	LEU	Α	88	37.029	14.622	-2.359	1.00 18.84	A
	MOTA	143	С	LEU	Α	88	38.815	18.632	-1.901	1.00 23.11	A
	MOTA	144	0	LEU	Α	88	37.999	19.146	-1.139	1.00 25.10	A
10	MOTA	145	N	GLY	Α	89	39.997	19.174	-2.149	1.00 24.09	A
	MOTA	146	CA	GLY		89	40.367	20.418	-1.507	1.00 24.27	Α
	ATOM	147	С	GLY	A	89	41.658	20.954	2.078	1.00 25.47	Α
	MOTA	148	0	GLY		89	42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	GLU		90	41.870	22.254	-1.906	1.00 26.22	A
15	ATOM	150	CA	GLU		90	43.064	22.924	-2.404	1.00 29.96	Α
15	ATOM	151	CB	GLU		90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU		90	42.267	23.038	-4.831	1.00 34.32	Α
	ATOM	153	CD	GLU		90	41.711	23.930	-5.927	1.00 38.27	A
	ATOM	154		GLU		90	40.590	24.456	-5.764	1.00 40.57	A
20	ATOM	155	OE2	GLU		90	42.398	24.110	-6.952	1.00 40.90	A
20	ATOM	156	C	GLU		90	43.711	23.768	-1.313	1.00 30.68	A
	ATOM	157	ō	GLU		90	43.049	24.574	-0.668	1.00 32.83	A
	ATOM	158	N	GLY		91	45.006	23.566	-1.104	1.00 29.66	Α
	ATOM	159	CA	GLY		91	45.724	24.332	-0.104	1.00 29.40	A
25	ATOM	160	C	GLY		91	46.795	25.151	-0.798	1.00 29.98	A
23	ATOM	161	ō	GLY		91	46.894	25.130	-2.028	1.00 28.16	Α
	ATOM	162	N	SER		92	47.605	25.870	-0.029	1.00 28.30	Α
	MOTA	163	CA	SER		92	48.653	26.681	-0.633	1.00 30.50	Α
	ATOM	164	СВ	SER		92	49.165	27.717	0.370	1.00 32.43	A
30	ATOM .	165	OG	SER		92	49.520	27.099	1.593	1.00 40.94	Α
	ATOM	166	C	SER		92	49.815	25.843	-1.164	1.00 29.77	A
	MOTA	167	0	SER		92	50.456	26.221	-2.143	1.00 30.46	Α
	ATOM	168	N	PHE	Α	93	50.087	24.703	-0.536	1.00 27.65	Α
	ATOM	169	CA	PHE		93	51.185	23.855	-0.995	1.00 26.34	Α
35	ATOM	170	CB.	PHE	A	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	Α	93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	A	93	52.283	25.909	1.392	1.00 29.96	A
	ATOM	173	CD2	PHE	A	93	53.949	25.613	-0.308	1.00 31.38	Α
	ATOM	174	CE1	PHE	Α	93	52.779	27.181	1.665	1.00 32.69	A
40	ATOM	175	CE2	PHE	Α	93	54.452	26.883	-0.044	1.00 32.63	A
	MOTA	176	CZ	PHE	Α	93	53.864	27.670	0.945	1.00 31.81	A
	ATOM	177	C	PHE	A	93	50.759	22.445	-1.365	1.00 25.39	A
	ATOM	178	0	PHE	A	93	51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER	Α	94	49.457	22.235	-1.519	1.00 23.63	A
45	ATOM	180	CA	SER	A	94	48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	CB	SER		94	49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER	Α	94	48.091	20.475	0.340	1.00 21.19	A
	ATOM	183	C	SER	Α	94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	0	SER	. A	94	46.795	21.882	-2.173	1.00 18.76	A
50	ATOM	185	N	THR	A	95	47.174	19.832	-3.038	1.00 19.38	A
	MOTA	186	CA	THR	A	95	45.840	19.637	-3.580	1.00 17.98	A
	MOTA	187	CB	THR	Α	95	45.818	19.818	-5.110	1.00 19.25	A
	MOTA	188	OG1	L THR	. A	95	46.196	21.162	-5.434	1.00 22.04	A
	MOTA	189	CG2	2 THR	Α	95	44.421	19.549	-5.661	1.00 17.61	A
55	MOTA	190	C	THR	A	95	45.455	18.201	-3.243	1.00 18.61	A
	ATOM	191	0	THR		95	46.212	17.264	-3.524	1.00 17.10	A A
	MOTA	192	N	VAL		96	44.295	18.024	-2.623	1.00 16.53	. A
	MOTA	193	CA	VAL		96	43.845	16.685	-2.266	1.00 16.05	A n
	MOTA	194	CB	VAL	Α	96	43.170	16.672	-0.886	1.00 16.32	A

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	ATOM	195	CG1	VAL	A	96	42.741	15.249	-0.532	1.00		A
	ATOM	196	CG2	VAL	Α	96	44.145	17.206	0.168	1.00	16.69	A
	ATOM	197	C	VAL	A	96	42.875	16.207	-3.335	1.00	16.42	A
	ATOM	198	o	VAL	Α	96	41.906	16.892	-3.665		16.47	A
5	ATOM	199	N	VAL	Α	97	43.157	15.033	-3.888	1.00	16.80	A
	MOTA	200	CA	VAL	Α	97	42.338	14.471	-4.949	1.00	16.72	A
	MOTA	201	CB	VAL	A	97	43.153	14.354	-6.255	1.00	18.43	A
	ATOM	202	CG1	VAL	Α	97	42.249	13.927	-7.404	1.00	19.69	Α
	ATOM	203	CG2	VAL	A	97	43.831	15.685	-6.569	1.00	17.84	A
10	ATOM	204	С	VAL		97	41.812	13.091	-4.583	1.00	16.77	A
	ATOM	205	0	VAL	Α	97	42.532	12.270	-4.014	1.00	17.13	A
	ATOM	206	N	LEU		98	40.545	12.845	-4.895	1.00	16.62	A
	MOTA	207	CA	LEU		98	39.947	11.548	-4.624	1.00	17.04	A
	ATOM	208	CB	LEU		98	38.424	11.633	-4.743	1.00	16.89	A
15	ATOM	209	CG	LEU		98	37.635	10.342	-4.508	1.00	19.46	A
15	ATOM	210		LEU		98	37.990	9.762	-3.146	1.00	20.07	A
	MOTA	211		LEU		98	36.143	10.627	-4.588	1.00	17.93	A
	ATOM	212	C	LEU		98	40.512	10.597	-5.677	1.00	17.38	A
	ATOM	213	ō	LEU		98	40.527	10.920	-6.863	1.00	18.60	A
20	ATOM	214	N	ALA		99	40.995	9.438	-5.246	1.00	17.13	A
20	ATOM	215	CA	ALA		99	41.570	8.466	-6.168	1.00	18.42	A
		216	CB	ALA		99	43.090	8.524	-6.105	1.00	14.76	A
	ATOM ATOM	217	C	ALA		99	41.102	7.055	-5.848	1.00	21.40	Α
		218	o	ALA		99	40.941	6.691	-4.679	1.00	22.52	A
25	MOTA		N			100	40.878	6.261	-6.888	1.00	19.77	A
25	MOTA	219	CA			100	40.459	4.884	-6.693		20.85	A
	ATOM	220	CB			100	39.202	4.585	-7.518		24.22	A
	ATOM	221	CG			100	38.608	3.205	-7.256	1.00	31.78	A
	MOTA	222				100	37.326	2.979	-8.048		36.24	A
20	MOTA	223	CD NE			100	36.213	3.818	-7.594	1.00	41.40	A
30	MOTA	224	CZ			100	35.566	3.662	-6.439	1.00	42.05	A
	ATOM	225		ARG			35.912	2.696	-5.598	1.00	40.67	A
	ATOM	226 227		ARG			34.559	4.468	-6.128	1.00	43.65	A
	MOTA		C			100	41.613	3.985	-7.129	1.00	18.63	A
25	MOTA	228	0			100	42.078	4.065	-8.271	1.00	19.49	Α
35	MOTA	229	И			101	42.102	3.157	-6.212		16.43	A
	ATOM	230	CA			101	43.196	2.246	-6.533	1.00	16.11	A
	ATOM	231 232	CB			101	43.774	1.637	-5.248		16.79	A
	MOTA	232	CG			101	44.917	0.657		1.00	16.51	A
40	ATOM	234	CD			101	45.501	0.115	-4.200	1.00	18.20	A
40	ATOM	235		GLU			44.733	-0.081	-3.239	1.00	18.32	A
	MOTA MOTA	236	-	GLU			46.725	-0.132	-4.150	1.00	17.14	A
	ATOM	237	C			101	42.625	1.152	-7.442	1.00	17.92	A
	ATOM	238	o			101	41.681	0.462	-7.069	1.00	18.02	Α
45	ATOM	239	N			102	43.198		-8.632	1.00	19.06	A
43		240	CA			102	42.718	0.025	-9.607		20.71	A
	ATOM	241	CB			102	43.569		-10.878		23.42	A
	ATOM		CG			102	43.531		-11.642		25.30	A
	ATOM	242 243		LEU			44.577		-12.748		27.88	A
50	ATOM	243		L DEC			42.140		-12.214		26.79	A
50	MOTA		CD			102	42.671	-1.418	-9.125	1.00	21.62	A
	ATOM	245	0			102	41.668	-2.103	-9.305		21.09	Α
	MOTA	246				103	43.753	-1.874	-8.507	1.00	19.38	A
	MOTA	247 248	N			103	43.836	-3.249	-8.035		20.87	A
e e	ATOM	249	CA CB			103	45.284	-3.571	-7.671		19.23	A
55	ATOM	250	CB			103	42.919		_		19.92	A
	ATOM	250 251	0			103	42.703	-4.815		1.00	20.38	A
	ATOM ATOM	251	N			103	42.361			1.00	18.12	A
		252	CA			104	41.517			1.00	17.15	A
	ATOM	255	CA	1111								

	ATOM	254	СВ	THR A	104	42.	212	-2.484	-3.717	1.00	19.54	A
	MOTA	255	OG1	THR A	104	42	456	-1.070	-3.773	1.00	19.26	A
	ATOM	256	CG2 ·	THR A	104	43.	. 536	-3.219	-3.529		17.02	A
	MOTA	257	С	THR A	104	40	.159	-2.247	-5.026		19.44	A
5	MOTA	258	0	THR A	104	39	.259	-2.648	-4.285		18.70	A
	ATOM	259	N	SER A	105	40	.034	-1.207	-5.847		19.65	A
	MOTA	260	CA	SER A	105	38	.819	-0.400	-5.967		19.37	Α
	MOTA	2,61	CB	SER A	105	37	.598	-1.304	-6.173		21.81	A
	ATOM	262	OG	SER A	105	. 36	.431	-0.539	-6.412		23.01	A
10	MOTA	263	C	SER A	105	38	.644	0.447	-4.701		18.99	A
	ATOM	264	0	SER A		37	.602	1.070	-4.488		18.66	A
	MOTA	265	N	ARG A	106		.674	0.468	-3.861		16.84	A
	MOTA	266	CA	ARG A	106		. 655	1.267	-2.634		16.21	A
	MOTA	267	CB	ARG A			.827	0.886	-1.723		16.41	A
15	MOTA	268	CG	ARG A			.619	-0.367	-0.906		15.49	A
•	MOTA	269	CD	ARG A			.887	-0.755	-0.170		17.43	A
	MOTA	270	NE	ARG A			.620	-1.792	0.824		20.47	A A
	ATOM	271	CZ	ARG A			.548	-2.568	1.371		20.24	A
	ATOM	272		ARG A			.821	-2.433	1.017		17.80 20.14	A
20	ATOM	273		ARG A			.198	-3.468	2.285		17.37	A
	ATOM	274	C	ARG A			.785	2.746	-2.981		17.75	A
	MOTA	275	0	ARG A			.514	3.103	-3.902		16.06	· A
	MOTA	276	N	GLU A			.085	3.599	-2.240		20.80	A
	MOTA	277	CA	GLU A			.156	5.039	-2.461 -2.337		22.93	A
25	MOTA	278	CB	GLU A			.779	5.694	-3.269		30.87	A
	MOTA	279	CG	GLU A			.711	5.171 5.975	-3.148		32.40	A
	MOTA	280	CD	GLU A			.431	6.939	-3.923		33.74	A
	ATOM	281		GLU F			.262 .608	5.654	-2.263		36.00	A
20	MOTA	282		GLU A			.053	5.678	-1.410		18.93	A
30	MOTA	283	C	GLU A			.891	5.427	-0.220		19.21	A
	ATOM	284	0	GLU F			.988	6.507	-1.852		16.70	A
	MOTA	285	N	TYR A			.883	7.209	-0.942		15.86	A
	MOTA	286	CA CB	TYR A			.325	6.728	-1.104		15.30	Α
25	MOTA	287 288	CG	TYR A			.593	5.328	-0.612		16.33	· A
35	ATOM ATOM	289	CD1				.765	5.066	0.746	1.00	16.36	A
	ATOM	290	CE1	•			.046	3.769	1.201	1.00	18.48	Α
	ATOM	291	CD2				.701	4.268	-1.511	1.00	13.25	A
	ATOM	292	CE2				.980	2.981	-1.075	1.00	17.28	A
40	ATOM	293	CZ		A 108		.152	2.736	0.276	1.00	19.17	A
40	ATOM	294	ОН		A 108		.440	1.461	0.688	1.00	19.38	A
	ATOM	295	C		A 108		.850	8.687	-1.292		16.80	A
	ATOM	296	ō .	TYR I	A 108	41	560	9.058	-2.431	1.00	15.22	A
	ATOM	297	N		A 109	42	1.132	9.528	-0.306		14.61	A
45	ATOM	298	CA		A 109	42	2.207	10.957	-0.539	1.00	14.30	Α
	ATOM	299	CB '		A 109	41	.671	11.726	0.661		14.78	A
	ATOM	300	С	ALA Z	A 109	43	3.713	11.136	-0.667		16.79	A
	ATOM	301	0	ALA	A 109	44	1.450	10.983	0.317		16.52	A
	ATOM	302	N	ILE 2	A 110	44	1.182	11.410	-1.881		14.80	A
50	ATOM	303	CA	ILE A	A 110	45	5:609	11.574	-2.093		15.80	A
	MOTA	304	CB	ILE :	A 110	4 6	5.065	10.863	-3.396		16.85	A
	MOTA	305		ILE .		47	7.550	11.098	-3.632		16.80	. A
	MOTA	306	CG1	ILE .	A 110		5.774	9.358	-3.284	1.00	17.76	A N
	ATOM	307	CD1	ILE .	A 110		5.308	8.513	-4.437		16.07	A
55	MOTA	308	С		A 110		5.004	13.045	-2.129		17.78	A A
	MOTA	309	0		A 110		5.534	13.813	-2.976	1.00	16.24 16.15	A
	MOTA	310	N		A 111		5.846	13.435	-1.177	1.00	17 20	A
	ATOM	311	CA		A 111		7.326	14.808	-1.100	1.00	17.20 17.41	A
	ATOM	. 312	CB	LYS	A 111	4	7.700	15.176	0.344	1.00	, 11.41	M

	MOTA	313	CG	LYS A	111	48.350	16.547	0.464	1.00 20.71	A
	MOTA	314	CD	LYS A	111	48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE	LYS A	111	47.288	17.381	2.598	1.00 29.46	A
	ATOM	316	NZ	LYS A	111	47.516	17.866	4.000	1.00 30.50	A
5	ATOM	317	C	LYS A	111	48.551	14.890	-1.994	1.00 16.41	A
	ATOM	318	0	LYS A	. 111	49.509	14.137	-1.813	1.00 18.20	Α
	ATOM	319 `	N	ILE A	112	48.509	15.798	-2.963	1.00 15.87	A
	MOTA	320	CA	ILE A	112	49.606	15.967	-3.907	1.00 17.28	A
	MOTA	321	CB	ILE A	112	49.079	15.911	-5.358	1.00 16.43	A
10	MOTA	322	CG2	ILE A	112	50.235	15.998	-6.341	1.00 15.12	A
	MOTA	323	CG1	ILE A	112	48.293	14.609	-5.565	1.00 16.82	A
	MOTA	324	CD1	ILE A	112	47.580	14.511	-6.904	1.00 18.47	A
	MOTA	325	С	ILE A	112	50.307	17.301	-3.663	1.00 19.03	A
	MOTA	326	0	ILE A	112	49.669	18.350	-3.635	1.00 19.15	A
15	MOTA	327	N	LEU A	113	51.622	17.245	-3.472	1.00 20.22	Α
	ATOM	328	CA	LEU A	113	52.416	18.442	-3.214	1.00 22.36	Α
	ATOM	329	CB	LEU P	113	52.995	18.397	-1.794	1.00 22.13	Α
	MOTA	330	CG	LEU A	113	52.042	18.063	-0.646	1.00 22.46	A
	MOTA	331	CD1	LEU A	113	51.866	16.557	-0.553	1.00 23.81	A
20	ATOM	332	CD2	LEU F	113	52.603	18.595	0.660	1.00 23.68	А
	ATOM	333	C	LEU P	113	53.560	18.547	-4.215	1.00 23.37	A
	ATOM	334	0	LEU A	113	54.300	17.586	-4.424	1.00 23.11	A
	ATOM	335	N	GLU A	114	53.706	19.714	-4.834	1.00 23.88	A
	MOTA	336	CA	GLU A	114	54.771	19.920	-5.806	1.00 26.00	A
25	ATOM	337	CB	GLU A	114	54.435	21.111	-6.706	1.00 27.74	A
	ATOM	338	CG	GLU A	114	55.533	21.452	-7.696	1.00 35.07	Α
	ATOM	339	CD	GLU A	114	55.220	22.696	-8.497	1.00 39.24	A
	ATOM	340	OE1	GLU A	114	54.808	23.703	-7.885	1.00 41.45	A
	ATOM	341	OE2	GLU A	114	55.395	22.670	-9.736	1.00 44.05	A
30	ATOM	342	С	GLU A	114	56.087	20.163	-5.067	1.00 24.37	Α
	ATOM	343	0	GLU A	114	56.186	21.071	-4.238	1.00 24.43	· A
	MOTA	344	N	LYS A	115	57.096	19.350	-5.360	1.00 24.10	A
	ATOM	345	CA	LYS A	115	58.376	19.493	-4.678	1.00 24.93	A
	ATOM	346	CB	LYS A	115	59.339	18.373	-5.103	1.00 23.72	Α
35	ATOM	347	CG	LYS A	115	59.139	17.080	-4.308	1.00 23.09	A
	ATOM	348	CD	LYS A	115	60.064	15.944	-4.743	1.00 21.92	A
	MOTA	349	CE		115		15.400	-6.117	1.00 22.42	A
	ATOM	350	NZ	LYS A	1115	60.447	14.150	-6.448	1.00 19.71	A
	MOTA	351	C	LYS A	1115	59.031	20.858	-4.868	1.00 26.87	- A
40	MOTA	352	0		115		21.469	-3.903	1.00 26.17	A
	MOTA	353	N	ARG A	1116		21.348	-6.102	1.00 28.73	A
	MOTA	354	CA		1116		22.638	-6.380	1.00 29.66	A
	MOTA	355	CB	ARG 2	116	59.533	22.980	-7.868	1.00 31.29	A
•	ATOM	356	CG		1116		24.361	-8.267	1.00 33.19	A
45	MOTA	357	CD	ARG A	116	61.368	24.710	-7.590	1.00 35.13	A
	MOTA	358	NB		A 116		23.612	-7.618	1.00 36.42	A
	MOTA	359	CZ		A 116		23.648	-7.009	1.00 36.18	A
	MOTA	360		ARG A			24.729	-6.332	1.00 36.12	A
	MOTA	361	NH2	ARG A			22.602	-7.067	1.00 35.77	A
50	ATOM	362	C		A 116		23.761	-5.519	1.00 29.70	A
	MOTA	363	0		A 116		24.515	-4.889	1.00 29.16	A
	MOTA	364	N		A 117		23.862	-5.472	1.00 27.22	A
	MOTA	365	CA		A 117		24.903	-4.681	1.00 26.33	A
	MOTA	366	CB		A 117		24.835	-4.848	1.00 28.41	A
55	MOTA	367	CG		A 117		26.005	-4.258	1.00 31.82	A
	MOTA	368		HIS .			27.249	-3.935	1.00 33.19	A A
	ATOM	369		HIS 2			25.974	-3.961	1.00 34.30	A n
	MOTA	370		HIS :			27.148	-3.480	1.00 34.58	A
	ATOM	371	NE2	HIS .	A 117	54.222	27.940	-3.455	1.00 35.18	A

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	MOTA	372	C I	HIS A 11	.7	5	7.477	24.780	-3.202		26.22	A
	ATOM	373	0 1	HIS A 1:	۱7	5	7.737	25.776	-2.534		25.67	A
	ATOM	374	N :	ILE A 1:	L8	5	7.469	23.554	-2.689		24.94	A
	ATOM	375	CA :	ILE A 1	L8 .	5	7.792	23.315	-1.285		23.94	A
5	ATOM	376	CB :	ILE A 1:	L8	5	7.711 .	21.812	-0.952		23.50	A
•	ATOM	377		ILE A 1	18	5	8.374	21.533	0.389		23.76	Α
	ATOM	378	_	ILE A 1		5	6.246	21.362	-0.959	1.00	24.42	A
	ATOM	379		ILE A 1		5	6.066	19.858	-0.834	1.00	28.06	A
		380		ILE A 1			9.195	23.821	`-0.958	1.00	23.78	A
10	MOTA	381	_	ILE A 1			9.402	24.495	0.048	1.00	23.49	A
10	ATOM		-	ILE A 1			0.153	23.489	-1.815	1.00	23.46	A
	ATOM	382		ILE A 1			1.534	23.913	-1.619	1.00	25.13	A
	MOTA	383		ILE A 1			2.467	23.250	-2.664	1.00	24.25	A
	ATOM	384		ILE A 1			3.858	23.890	-2.617		22.47	A
	ATOM	385						21.738	-2.395		25.05	A
15	ATOM	386		ILE A 1			52.540	20.945	-3.439		24.62	A
	MOTA	387		ILE A 1			53.327	25.435	-1.705		25.96	' A
	ATOM	.388		ILE A 1			51.667		-0.872		24.78	A
	MOTA	389	_	ILE A 1			52.330	26.051			27.67	A
	MOTA	390		LYS A 1			51.028	26.039	-2.704		30.29	. A
20	MOTA	391		LYS A 1			51.100	27.489			32.34	A
	MOTA	392	CB	LYS A 1	20		50.242	27.940	-4.060		39.30	A
	MOTA	393		LYS A 1			50.674	27.407	-5.409			A
	ATOM	394		LYS A 1			59.765	27.950	-6.512		45.19	A
	ATOM	395	CE	LYS A 1	20		58.294	27.636	-6.218		46.48	
25	ATOM	396	NZ	LYS A 1	20		57.363	28.155	-7.252		46.49	A _.
	ATOM	397	C	LYS A 1	20	• 1	60.647	28.247	-1.638		30.89	A
	ATOM	398	0	LYS A 1	20		61.303	29.198	-1.217		32.48	A
	ATOM	399	N	GLU A 1	21		59.527	27.825	-1.055		29.82	A
	ATOM	400	CA	GLU A 1	21		58.986	28.488	0.128		30.33	A
30	ATOM	401	СВ	GLU A 1			57.455	28.416	0.117		33.04	A
50	ATOM	402	CG	GLU A 1	.21		56.794	29.021	-1.120		36.45	A
	ATOM	403	CD	GLU A			57.221	30.456	-1.373		39.88	A
	ATOM	404		GLU A			57.200	31.264	-0.420		40.53	A
	ATOM	405		GLU A			57.573	30.778	-2.529		43.24	A
35	ATOM	406		GLU A			59.511	27.930	1.451		30.37	A
. 33		407	0	GLU A			58.946	28.204	2.513	1.00	31.24	A
	MOTA	. 408	Ŋ	ASN A			60.588	27.151	1.390		29.03	A
	MOTA	409	CA	ASN A			61.183	26.573	2.594		28.46	A
	MOTA	410	CB	ASN A			61.836	27.673	3.436	1.00	31.28	A
40	ATOM		CG	ASN A			62.945	28.395	2.698	1.00	34.12	А
40	ATOM	411		ASN A			62.697	29.143	1.754	1.00	35.57	A
	MOTA	412		ASN A			64.181	28.169	3.127	1.00	0 35.73	A
	MOTA	413		ASN A			60.157	25.835	3.456	_	0 26.89	Α
	ATOM	414	C	ASN A			60.085	26.055			0 27.23	A
	MOTA	415	0				59.375	24.955	2.842		0 23.99	, A
45	ATOM	416	И	LYS A			58.358	24.210			0 22.43	A
	MOTA	417	CA	LYS A				24.248		1.0	0 21.97	A
	MOTA	418		LYS A			57.031	25.645			0 25.68	A
	MOTA	419		LYS A			56.475	26.354			0 27.54	A
	MOTA	420		LYS A			56.253			_	0 31.30	A
50	MOTA	421	CE	LYS A			55.822	27.796			0 33.21	A
	MOTA	422	NZ	LYS A			55.756				0 22.20	A
	MOTA	423	C	LYS A			58.748				0 22.50	A
	MOTA	424	0	LYS A			57.924			_	0 22.50	A
	MOTA	425	N	VAL A			59.997			_	0 20.35	A
55	ATOM	426	CA	VAL A			60.439			_	0 19.43	A
	MOTA	427	CB	VAL A			61.922			_	10 10 60	
	ATOM	428		VAL A			62.346				0 18.69	A
	ATOM	429	CG2	VAL A	124		62.104			_	0 18.21	A
	MOTA	430		VAL A			60.236	20.561	5.163	3 1.0	0 19.53	A

	ATOM	431	0	VAL A 124	59.841	19.418	5.385	1.00 20.02	A
	ATOM	432		PRO A 125	60.513	21.422	6.159	1.00 20.01	A
	ATOM	433		PRO A 125	61.178	22.738	6.118	1.00 18.69	A
		434		PRO A 125	60.318	20.979	7.544	1.00 19.88	A
•	ATOM	435		PRO A 125	60.793	22.180	8.363	1.00 19.95	A
5	MOTA			PRO A 125	61.839	22.805	7.479	1.00 18.85	A
	ATOM	436		PRO A 125	58.848	20.642	7.824	1.00 19.76	A
	ATOM	437			58.544	19.700	8.550	1.00 16.99	A
	MOTA	438		PRO A 125	57.947	21.418	7.235	1.00 18.98	A
	MOTA	439		TYR A 126		21.220	7.435	1.00 21.97	A
10	MOTA	440		TYR A 126	56.516	22.448	6.933	1.00 25.17	A
	MOTA	441		TYR A 126	55.752	23.690	7.748	1.00 30.98	A
	ATOM	442	CG	TYR A 126	56.040			1.00 33.95	A
	MOTA	443		TYR A 126	55.438	23.886	8.991	1.00 36.60	A
	MOTA	444		TYR A 126	55.721	25.015	9.763	1.00 35.43	A
15	MOTA	445			56.938	24.657	7.292		Ä
	ATOM	446	CE2	TYR A 126	57.231	25.792	8.058	1.00 37.20	
	MOTA	447	CZ	TYR A 126	56.618	25.962	9.291	1.00 37.40	A
	MOTA	448	OH	TYR A 126	56.903	27.073	10.052	1.00 40.85	A
	ATOM	449	С	TYR A 126	55.990	19.956	6.762	1.00 21.35	A
20	MOTA	450	0	TYR A 126	55.265	19.175	7.383	1.00 20.49	A
	ATOM	451	N	VAL A 127	56 [.] .354	19.746	5.501	1.00 18.16	A
	ATOM	452	CA	VAL A 127	55.892	18.562	4.790	1.00 17.58	A
	ATOM	453	CB	VAL A 127	56.308	18.596	3.308	1.00 17.45	Α
	ATOM	454		VAL A 127 '	55.786	17.350	2.600	1.00 17.97	A
25	ATOM	455		VAL A 127	55.751	19.850	2.641	1.00 14.90	A
23	MOTA	456	C	VAL A 127	56.459	17.306	5.448	1.00 18.39	A
	MOTA	457	Ö	VAL A 127	55.769	16.298	5.583	1.00 18.14	A
	ATOM	458	N	THR A 128	57.716	17.381	5.869	1.00 17.50	A
	ATOM	459	CA	THR A 128	58.375	16.260	6.530	1.00 18.54	. A
20		460	CB	THR A 128	59.861	16.586	6.805	1.00 18.01	A
30	MOTA	461		THR A 128	60.537	16.804	5.559	1.00 21.14	A
	ATOM		CG2		60.536	15.446	7.545	1.00 17.95	Α
	ATOM	462	C	THR A 128	57.676	15.941	7.856	1.00 19.49	A
	MOTA	463		THR A 128	57.438	14.776	8.179	1.00 18.76	A
	MOTA	464	0	ARG A 129	57.345	16.981	8.619	1.00 19.60	A
35	MOTA	465	N		56.673	16.804	9.904	1.00 20.12	A
•	ATOM	466	CA	ARG A 129	56.534	18.144	10.621	1.00 21.33	A
	MOTA	467	CB	ARG A 129	55.948	18.029	12.023	1.00 28.02	A
	ATOM	468	CG	ARG A 129		19.404	12.597	1.00 31.25	A
	MOTA	469	CD	ARG A 129	55.721	20.205	12.560	1.00 37.78	A
40	MOTA	470	NE	ARG A 129	56.940	21.524	12.391	1.00 40.10	A
	ATOM	471	CZ	ARG A 129	56.962	22.197	12.239	1.00 40.03	A
	MOTA	472		ARG A 129	55.828		12.233	1.00 44.58	A
•	ATOM	473		ARG A 129	58.119	22.170	9.729	1.00 20.08	A
	ATOM	474	С	ARG A 129	55.288	16.186	10.496		A
45	MOTA	475	0	ARG A 129	54.891	15.305	8.724	1.00 18.79	A
	ATOM	476	N	GLU A 130	54.553	16.654		1.00 20.10	. A
	ATOM	477	. CA	GLU A 130	53.222		8.454	1.00 19.92	A
	MOTA	478	CB	GLU A 130	52.638		7.183	1.00 19.32	A
	MOTA	479	CG	GLU A 130	51.350		6.708		A
50	ATOM	480		GLU A 130	50.581	_	5.707	1.00 29.72	A
	ATOM	481	OE1	GLU A 130	51.216		4.814	1.00 33.46	
	ATOM	482		2 GLU A 130	49.339		5.807	1.00 30.74	A A
	ATOM	483	С	GLU A 130	53.301		8.295	1.00 19.81	A
	MOTA	484		GLU A 130	52.553		8.935	1.00 18.37	A.
55	MOTA	485		ARG A 131	54.219			1.00 20.41	A
	MOTA	486		ARG A 131	54.397	12.735		1.00 22.45	A
	MOTA	487		ARG A 131	55.442	12.511	6.098	1.00 25.16	A
	MOTA	488		ARG A 131	55.742	11.043	5.840	1.00 28.75	A
	ATOM	489		ARG A 131	56.736		4.708	1.00 33.75	A
	ATOM								

	ATOM	490	NE	ARG	A	131	57.020	9.415	4.520	1.00 40.07	A
	ATOM	491	CZ	ARG	A	131	57.756	8.915	3.532	1.00 43.07	A
	ATOM	492	NH1	ARG	Α	131	58.293	9.721	2.625	1.00 44.91	A
	ATOM	493	NH2	ARG	Α	131	57.955	7.606	3.449	1.00 44.45	A
5	ATOM	494	С	ARG	Α	131	54.820	11.982	8.466	1.00 23.24	A
	MOTA	495	0	ARG	A	131	54.241	10.948	8.804	1.00 23.86	A
	ATOM	496	N	ASP	Α	132	55.831	12.497	9.160	1.00 21.99	A
	ATOM	497	CA	ASP	Α	132	56.318	11.850	10.370	1.00 22.04	A
	ATOM	498	СВ	ASP	Α	132	57.570	12.564	10.888	1.00 23.72	A
10	MOTA	499	CG	ASP			58.750	12.442	9.932	1.00 27.77	A
	ATOM	500		ASP			58.681	11.620	8.989	1.00 27.34	A
	ATOM	501		ASP			59.753	13.163	10.128	1.00 28.70	A
	ATOM	502	C	ASP			55.258	11.772		1.00 21.69	A
	ATOM	503	o	ASP			55.077	10.723	12.092	1.00 22.75	A
15	ATOM	504	N	VAL			54.551	12.868		1.00 19.54	A
•	ATOM	505	CA	VAL			53.525	12.843		1.00 18.52	A
	ATOM	506	CB	VAL			52.908	14.244		1.00 19.26	A
	ATOM	507		VAL			51.708	14.135		1.00 18.79	A
	ATOM	508		VAL			53.953	15.180		1.00 18.80	A
20	ATOM	509	C	VAL			52.419	11.854		1.00 19.46	A
20	ATOM	510	o	VAL			52.073	10.991		1.00 19.94	A
	ATOM	511	N	MET			51.878	11.957		1.00 19.15	A
	ATOM	512	CA	MET			50.807	11.052		1.00 21.25	A
	ATOM	513	CB	MET			50.309	11.381		1.00 17.34	A
25	ATOM	514	CG	MET			49.615	12.730		1.00 20.00	A
25	ATOM	515	SD	MET			48.643	12.952		1.00 24.21	A
	ATOM	516	CE	MET			47.033	12.434		1.00 23.20	A
	ATOM	517	C	MET			51.203	9.582		1.00 22.43	A
		517	0	MET			50.384	8.741		1.00 23.82	A
20	ATOM		N			135	52.454	9.273		1.00 23.09	A
30	ATOM	519 520				135	52.939	7.895		1.00 26.13	A
	ATOM	520	CA CB			135	54.356	7.798		1.00 26.17	A
	ATOM	521				135	54.383	8.177		1.00 31.91	. A
	MOTA	522	OG				52.957	7.358		1.00 26.58	A
25	MOTA	523	C			135 135	52.926	6.148		1.00 26.42	A
35	ATOM	524	0				53.014	8.261		1.00 25.65	A
	ATOM	525	N			136	53.014	7.870		1.00 27.47	A
	ATOM	526	CA			136	53.823	8.914		1.00 27.97	A
	ATOM	527	CB			136	55.283	9.082		1.00 32.00	A
40	ATOM	528	CG			136	55.904	10.218		1.00 32.00	A
40	ATOM	529	CD			136	55.602	10.073		1.00 36.11	A
	ATOM	530	NE			136 c	55.867	10.990		1.00 30.11	A
	MOTA	531	CZ			136	56.449	12.132		1.00 40.55	A
	ATOM	532		ARG			55.540	10.769		1.00 36.72	A
4.5	MOTA	533		ARG						1.00 36.72	A
45	ATOM	534	C			136	51.667				A
	ATOM	535	0			136	51.516	7.121		1.00 27.06 1.00 24.77	. A
	MOTA	536	N			137	50.655	8.235		1.00 24.77	A
	ATOM	537	CA			137	49.294	8.162		1.00 24.70	A
	ATOM	538	CB			137	48.483	9.363			A
50	ATOM	539	CG			137	49.050	10.760		1.00 26.67	A
	MOTA	540		LEU			48.075	11.813		1.00 27.25 1.00 27.09	A
	ATOM	541		LEU			49.279				A
	MOTA	542	C			137	48.592	6.868		1.00 25.20	A
	ATOM	543	0			137	48.619			1.00 25.99	A
55	ATOM	544	N			138	47.971			1.00 21.89	A
	ATOM	545	CA			138	47.239			1.00 21.35	
	MOTA	546	CB			138	48.124			1.00 22.14	A
	MOTA	547	CG			138	47.432			1.00 24.90	A
	MOTA	548	OD1	. ASP	Α	138	46.631	2.423	3 14.241	1.00 24.78	A

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	ATOM	549	OD2	ASP A	138	4	17.691	1.443	15.897		25.39	Α
	MOTA	550	C	ASP A	138	4	6.031	4.991	16.138		20.47	Α
	ATOM	551		ASP A	138	4	15.967	4.248	17.118	1.00	19.06	Α
	ATOM	552	-	HIS A		4	15.075	5.852	15.810	1.00	18.27	Α
5	MOTA	553		HIS A			13.869	6.016	16.606	1.00	18.21	A
)				HIS A			14.096	7.157	17.612	1.00	15.84	A
	MOTA	554		HIS A			12.985	7.332	18.600		15.24	Α
	MOTA	555						6.964	19.900		13.97	A
	MOTA	556		HIS A			12.884		18.280		14.74	A
	MOTA	557		HIS A			41.791	7.943			14.19	A
10	MOTA	558		HIS A			41.002	7.944	19.341		14.15	A ·
	MOTA	559	NE2	HIS A	139	•	41.641	7.356	20.336			A
	MOTA	560		HIS A			42.715	6.330	15.654		18.50	
	ATOM	561	0	HIS A	139	•	42.879	7.080	14.693		20.80	A
	ATOM	562	N	PRO A	140		41.527	5.767	15.913		18.32	A
15	ATOM	563	CD	PRO A	140		41.143	4.984	17.100		16.71	A
~~	ATOM	564		PRO A	140		40.367	6.001	15.048		17.43	A
	ATOM	565	CB	PRO A			39.273	5.157	15.704	1.00	16.64	A
		566		PRO A			39.643	5.204	17.152	1.00	18.43	A
	MOTA		C	PRO A			39.914	7.441	14.803	1.00	18.77	A
•	MOTA	567		PRO A			39.207	7.695	13.831	1.00	19.88	A
20	ATOM	568	0				40.301	8.381	15.664		17.14	Α
	MOTA	569	N	PHE A			39.874	9.767	15.477		16.42	A
	MOTA	570	CA	PHE A			39.568	10.422	16.836		14.60	A
	MOTA	571	CB	PHE A				9.817	17.556		15.26	A
	MOTA	572	CG	PHE A			38.386				14.78	A
25	MOTA	573		PHE A			37.335	9.234	16.842		13.70	A
	MOTA	574		PHE A			38.297	9.880	18.942		16.94	A
	MOTA	575		PHE A			36.215	8.727	17.502			A
	MOTA	576	CE2	PHE A	141		37.178	9.375	19.615		15.75	A
	ATOM	57 7	CZ	PHE A	141		36.135	8.799	18.893		16.89	
30	ATOM	578	С	PHE A	141		40.857	10.641	14.694		16.15	A
-	ATOM	579	0	PHE A	141		40.799	11.871	14.761		17.35	A
	ATOM	580	N	PHE A			41.748	10.011	13.941		15.88	A
	ATOM	581	CA	PHE A			42.727	10.756	13.154	1.00	17.89	Α
	MOTA	582	CB	PHE A			44.115	10.645	13.793		17.57	A
25	ATOM	583	CG	PHE A			44.240	11.371	15.103	1.00	0 18.74	A
35		584		PHE A			44.559	12.726	15.135	1.00	0 17.77	A
•	MOTA			PHE A			43.997	10.711	16.304	1.0	0 18.74	A
	MOTA	585		PHE A			44.632	13.417	16.347	1.0	0 15.77	A
•	MOTA	586					44.065	11.393	17.522	1.0	0 17.56	A
	MOTA	587		PHE A			44.383	12.747	17.542		0 17.14	A
40	MOTA	588	CZ	PHE A			42.793	10.231	11.729		0 19.12	` A
	MOTA	589	C	PHE P				9.030	11.504		0 20.01	A
	MOTA	590	0	PHE A			42.659	11.135	10.769		0 18.72	A
	MOTA	591	И	VAL A			42.978		9.371		0 18.52	A
	ATOM	592	CA	VAL A	A 143		43.102	10.735			0 20.66	A
45	MOTA	593	CB	VAL	A 143		43.294					A
	MOTA	594	CG1	VAL A	A 143		43.843	11.521	7.080		0 21.29	A
	MOTA	595	CG2	VAL A	A 143		41.958	12.673			0 22.97	
	ATOM	596		VAL A	A 143		44.342	9.865	9.330		0 18.68	A
	ATOM	597			A 143		45.355	10.199			0 18.42	A,
50	ATOM	598			A 144		44.259	8.745	8.623	1.0	0 18.30	A
20	MOTA	599			A 144		45.384	7.824	8.535		0 18.78	A
		600			A 144		44.889	6.373			0 22.27	A
	MOTA	601			A 144		46.017	5.340			0 29.72	A
	ATOM				A 144		45.491	3,912		1.0	0 34.16	A
	ATOM	602			A 144 A 144		46.631				0 37.67	A
55	ATOM	603					46.138				0 39.02	A
	ATOM	604			A 144		46.192				0 18.53	Α
	MOTA	605			A 144		45.643				0 18.18	A
	MOTA	606			A 144						0 16.79	A
	MOTA	607	N	LEU	A 145		47.502	7.816	, ,,,,,,			_

	ATOM	608	CA	LEU A 145	48.411	7.900	6.251	1.00 17.45	A
									70
	ATOM	609	CB	LEU A 145	49.686	8.653	6.641	1.00 18.82	A
	ATOM	610	CG	LEU A 145	50.734	8.902	5.549	1.00 20.23	A
	ATOM	611	CD1	LEU A 145	51.836	9.799	6.093	1.00 18.83	A
5	MOTA	612	CD2	LEU A 145	51.317	7.581	5.069	1.00 19.79	A
	ATOM	613	C	LEU A 145	48.739	6.450	5.907	1.00 19.19	A
	MOTA	614	0	LEU A 145	49.451	5.772	6.659	1.00 17.36	A
	ATOM	615	N	TYR A 146	48.215	5.972	4.782	1.00 17.28	A A
	MOTA	616	CA	TYR A 146	48.444	4.593	4.358	1.00 17.57	A
10	ATOM	617	CB	TYR A 146	47.288	4.098	3.486	1.00 17.74	A
	MOTA	618	CG	TYR A 146	45.981	3.926	4.214	1.00 17.50 1.00 16.50	A
	MOTA	619	CD1	TYR A 146	45.099	4.995	4.377	1.00 16.50	A
	MOTA	620	CE1		43.881	4.827	5.039		A
	ATOM	621	CD2	TYR A 146	45.620	2.686	4.735	1.00 18.28	A
15	ATOM	622	CE2	TYR A 146	44.411	2.506	5.399	1.00 19.84 1.00 17.53	A
	MOTA	623	CZ	TYR A 146	43.547	3.576	5.544	1.00 17.53	A
	MOTA	624	ОН	TYR A 146	42.342	3.376	6.169		A
	MOTA	625	С	TYR A 146	49.735	4.376	3.582	1.00 18.72 1.00 19.51	A
	ATOM	626	0	TYR A 146		3.338	3.715	1.00 19.31	A
20	MOTA	627	И	PHE A 147		5.350	2.765	1.00 18.09	A
	MOTA	628	CA	PHE A 147		5.203	1.952	1.00 17.20	A
•	MOTA	629	CB	PHE A 147		4.258	0.783	1.00 10.77	A
	MOTA	630	CG	PHE A 147		4.699	-0.070	1.00 17.73	A
	MOTA	631		PHE A 147		5.752	-0.975	1.00 18.07	A
25	ATOM	632		PHE A 147		4.075	0.053	1.00 19.62	A
	MOTA	633		PHE A 147		6.178	-1.742	1.00 13.52	A
	MOTA	634	CE2	PHE A 147		4.492	-0.710	1.00 19.27	Α.
	MOTA	635	CZ	PHE A 147		5.546	-1.610	1.00 17.13	A
	MOTA	636	C	PHE A 147		6.533	1.395	1.00 14.43	A
30	MOTA	637	0	PHE A 147		7.528	1.452	1.00 17.12	A
	MOTA	638	И	THR A 148		6.534	0.854 0.232	1.00 17.12	A
	MOTA	639	CA	THR A 148		7.718	1.197	1.00 21.51	A
	MOTA	640	CB	THR A 148		8.531	1.537	1.00 18.83	Α
	MOTA	641	OG:			7.760 8.897	2.472	1.00 19.60	A
35	ATOM	642	ĊG:			7.262	-0.946	1.00 20.31	A
	MOTA	643	С	THR A 14		6.124	-0.991	1.00 18.94	A
	MOTA	644	0	THR A 14		8.149	-1.916	1.00 19.16	A
	MOTA	645	N	PHE A 14		7.877	-3.073	1.00 18.01	A
	MOTA	646	CA			6.801	-3.989	1.00 17.23	A
40	MOTA	647	СВ	PHE A 14		7.144	-4.544	1.00 16.88	A
	ATOM	648	CG	PHE A 14		7.888	-5.712	1.00 18.58	A
	MOTA	649		1 PHE A 14		6.668	-3.927		A
	MOTA	650		2 PHE A 14		8.149	-6.267	1.00 19.26	A
	MOTA	651		1 PHE A 14		6.923	-4.470		. A
45	MOTA	652		2 PHE A 14		7.663	-5.642		Α
	MOTA	653				9.205	-3.774		A
	MOTA	654		PHE A 14	₹	10.200	-3.376		A
	ATOM	655		PHE A 14		9.241	-4.782		A
	MOTA	656		GLN A 15		10.481	-5.497		A
50		657			*	11.347	-4.739	and the second s	A
	ATOM	658				10.645	-4.414		A
	ATOM	659			-	11.558	-3.692	1.00 29.02	A
	ATOM	660		GLN A 15		12.353	-4.321	1.00 27.05	A
	MOTA	661		2 GLN A 1:	-	11.449		1.00 26.47	A
55		662		GLN A 1:				1.00 23.88	A
	MOTA	663		GLN A 1:				3 1.00 24.79	A
	MOTA	664		ASP A 1	· _			1.00 25.88	A
	MOTA	66!							. A

	ATOM	667	CB .	ASP A 1	51	56.437	11.126	-10.199	1.00 24.54	Α
	ATOM	668	CG	ASP A 1	51	55.544	12.336	-10.064	1.00 24.95	A
	ATOM	669	OD1	ASP A 1	51	56.005	13.379	-9.561	1.00 22.44	Α
	ATOM	670	-	ASP A 1		54.369	12.242	-10.490	1.00 25.72	Α
5	ATOM	671		ASP A 1		58.515	12.203	-9.220	1.00 28.63	A
,	ATOM	672		ASP A 1		58.890	12.780	-8.194	1.00 27.83	A ·
		673		ASP A 1		58.934		-10.426	1.00 29.21	A
	MOTA			ASP A 1		59.907		-10.562	1.00 31.88	A
	ATOM	674	CA			60.325		-12.026	1.00 33.94	A
	MOTA	675	CB	ASP A 1				-12.557	1.00 38.88	A
10	MOTA	676		ASP A 1		61.033			1.00 39.67	A
	MOTA	677		ASP A 1		61.817		-11.791	1.00 33.07	A
	MOTA	678		ASP A 1		60.817		-13.738		A
	MOTA	679	С	ASP A 1		59.487		-10.013	1.00 30.90	A
	MOTA	680	0	ASP A 1	.52	60.316	15.735	-9.482	1.00 31.69	
15	ATOM	681	N	GLU A 1		58.207		-10.107	1.00 29.44	A
	ATOM	682	CA	GLU A 1	.53	57.767	16.632	-9.646	1.00 28.69	A
	ATOM	683	CB	GLU A 1	.53	56.984		-10.766	1.00 32.90	A
	ATOM	684	CG	GLU A 1	.53	57.451		-12.183	1.00 40.57	A
	MOTA	685	CD	GLU A 1	.53	56.920	15.643	-12.675	1.00 45.78	A
20	ATOM	686	OE1	GLU A 1		55.682	15.482	-12.760	1.00 48.91	A
20	MOTA	687	OE2	GLU A 1	53	57.736	14.747	-12.979	1.00 48.95	Α
-	MOTA	688	C	GLU A 1		56.929	16.683	-8.372	1.00 26.43	A
	MOTA	689	ō	GLU A 1		56.947	17.688	-7.660	1.00 25.08	A
	MOTA	690	N	LYS A 1		56.205	15.610	-8.069	1.00 22.39	A
25	ATOM	691	CA	LYS A		55.318	15.631	-6.912	1.00 21.43	A
25		692	CB	LYS A 1		53.861	15.628	-7.398	1.00 20.33	A
	ATOM			LYS A		53.505	16.716	-8.403	1.00 21.92	A
	MOTA	693	CG	LYS A		52.211	16.375	-9.146	1.00 19.70	A
	MOTA	694	CD			51.775		-10.077	1.00 20.04	A
	MOTA	695	CE	LYS A		50.631		-10.951	1.00 19.97	A
30	MOTA	696	NZ	LYS A				-5.881	1.00 20.43	A
	ATOM	697	C	LYS A		55.458	14.522	-6.173	1.00 21.13	A
	ATOM	698	0	LYS A		55.949	13.426		1.00 21.13	A
	ATOM	699	N	LEU A		54.985	14.832	-4.676	1.00 19.10	Α
	ATOM	700	CA	LEU A		54.950	13.900	-3.553	1.00 19.65	A
35	ATOM	701	CB	LEU A		55.362	14.588	-2.252	1.00 19.03	A
	ATOM	702	CG	LEU A	155	56.740	15.234			A
	MOTA	703	CD1	LEU A	155	56.848	15.918	-0.770	1.00 23.42	
	MOTA	704	CD2	LEU A :	155	57.816	14.174		1.00 23.08	A
	MOTA	705	С	LEU A	155	53.478	13.507	-3.427	1.00 18.87	A
40	MOTA	706	0	LEU A	155	52.600	14.348	-3.620	1.00 18.61	A
	ATOM	707	N '	TYR A	156	53.209	12.249	-3.091	1.00 15.02	A
	MOTA	708	CA	TYR A	156	51.834	11.783	-2.1934	1.00 16.29	A
	ATOM	709	CB	TYR A	156 [°]	51.470	10.769	-4.029	1.00 14.20	
	ATOM	710	CG	TYR A		51.603	11.273	-5.449	1.00 17.29	A
45	ATOM	711		TYR A	156	52.857	11.429	-6.045	1.00 16.46	A
73	ATOM	712		TYR A		52.978			1.00 18.68	A
	ATOM	713		TYR A		50.474			1.00 16.43	A
		714		TYR A		50.583			1.00 16.31	A
	MOTA	715	CEZ	TYR A		51.835			1.00 18.17	A
	MOTA			TYR A		51.941				
50	ATOM	716	ОН			51.657				
	ATOM	717	C	TYR A		52.412				
	MOTA	718	0	TYR A		50.678				
	MOTA	719	N	PHE A						
	MOTA	720	CA	PHE A		50.385		_		
55	MOTA	721	CB	PHE A		50.324				
	MOTA	722	CG	PHE A		51.631				
	MOTA	723		PHE A		52.821				
	MOTA	724		PHE A		51.664				
	ATOM	725	CE1	PHE A	157	54.025	12.92	1.585	1.00 22.00	, А

	ATOM	726	CE2	PHE A	A 157	52.865	14.500	2.982	1.00 22.18	A
	MOTA	727	CZ	PHE A	A 157	54.045	14.045	2.405	1.00 21.27	A
	ATOM	728	С	PHE A	A 157	49.016	10.308	0.404	1.00 16.52	A
	ATOM	729	0	PHE A	A 157	48.029	10.979	0.110	1.00 17.32	A
5	ATOM	730	N	GLY A	A 158	48.953	9.002	0.644	1.00 15.97	A
	ATOM	731	CA	GLY A	A 158	47.684	8.299	0.572	1.00 16.13	Α
	MOTA	732	C	GLY A	A 158	47.000	8.383	1.920	1.00 14.94	A
	MOTA	733	0	GLY A	A 158	47.445	7.756	2.879	1.00 16.28	Α
	MOTA	734	N	LEU Z	A 159	45.915	9.145	1.989	1.00 13.50	A
10	MOTA	735	CA	LEU.	A 159	45.191	9.340	3.241	1.00 15.20	A
	MOTA	736	CB	LEU 2	A 159	45.031	10.835	3.517	1.00 14.20	A
	ATOM	737	CG	LEU I	A 159	46.270	11.726	3.385	1.00 19.00	A
	MOTA	738	CD1	LEU Z	A 159	45.847	13.188	3.477	1.00 17.12	A
	ATOM	739	CD2	LEU A	A 159	47.275	11.390	4.471	1.00 14.71	, A
15	MOTA	740	C	LEU 2	A 159	43.809	8.716	3.232	1.00 15.53	A
	MOTA	741	0	LEU I	A 159	43.232	8.472	2.177	1.00 16.05	A
	ATOM	742	N	SER 2	A 160	43.268	8.469	4.418	1.00 15.86	A
	MOTA	743	CA	SER I	A 160	41.932	7.917	4.498	1.00 19.01	A
	ATOM	744	CB	SER 3	A 160	41.566	7.582	5.949	1.00 22.90	A
20	MOTA	745	OG	SER .	A 160	41.901	8.629	6.833	1.00 24.18	A
	MOTA	746	С	SER .	A 160	40.987	8.968	3.924	1.00 20.43	A
	ATOM	747	0	SER .	A 160	41.213	10.173,	4.062	1.00 19.96	A
	MOTA	748	N	TYR .	A 161	39.945	8.508	3.250	1.00 19.20	A
	ATOM	749	CA	TYR .	A 161	38.975	9.406	2.644	1.00 20.37	A
25	ATOM	750	CB	TYR .	A 161	38.471	8.785	1.332	1.00 20.00	. A
	MOTA	751	CG	TYR	A 161	37.314	9.502	0.666	1.00 20.72	A
	MOTA	752	CD1	TYR .	A 161	37.222	10.895	0.682	1.00 18.22	A
	MOTA	753	CE1	TYR	A 161	36.180	11.557	0.029	1.00 22.24	A
	MOTA	754	CD2	TYR	A 161	36.333	8.784	-0.020	1.00 20.53	A
30	MOTA	755	CE2	TYR	A 161	35.287	9.436	-0.678	1.00 24.24	A
	ATOM	756	CZ	TYR	A 161	35.218	10.822	-0:648	1.00 22.32	A
	ATOM	757	OH	TYR	A 161	34.194	11.471	-1.298	1.00 23.03	A
	MOTA	758	С	TYR	A 161	37.812	9.681	3.598	1.00 20.14	Α
	MOTA	759	0	TYR	A 161	36.959	8.819	3.810	1.00 19.53	A
35	MOTA	760	И	ALA	A 162	37.791	10.880	4.178	1.00 19.92	Α
	MOTA	761	CA	ALA	A 162	36.721	11.271	5.099	1.00 21.07	A
	MOTA	762	CB	ALA	A 162	37.187	12.419	6.002	1.00 19.60	A
	ATOM	763	C	ALA	A 162	35.542	11.712	4.238	1.00 22.07	A
	ATOM	764	0	ALA	A 162	35.436	12.875	3.860	1.00 20.66	A
40	ATOM	765	И	LYS	A 163	34.653	10.769	3.945	1.00 23.27	A
	ATOM	766	CA	LYS	A 163	33.503	11.017	3.080	1.00 27.12	Α
	MOTA	767	CB	LYS	A 163	32.663	9.741	2.963	1.00 29.68	A
	ATOM	768	CG	LYS	A 163	33.455	8.524	2.515	1.00 37.67	A
	MOTA	769	$^{\mathtt{CD}}$		A 163	32.556	7.310	2.321	1.00 42.24	A
45	MOTA	770	CE		A 163		6.034	2.185	1.00 44.48	A
	MOTA	771	NZ	LYS	A 163	34.143	5.735	3.430	1.00 44.88	A
	ATOM	772	C	LYS	A 163	32.581	12.186	3.411	1.00 25.78	A
	MOTA	773	0	LYS	A 163	32.103	12.863	2.506	1.00 26.53	A
	ATOM	774	N	ASN	A 164		12.441	4.689	1.00 24.57	A
50	ATOM	775	CA		A 164		13.522	5.033	1.00 23.77	A
	ATOM	776	CB	ASN	A 164		13.129	6.265	1.00 25.02	A
	ATOM	777	CG		A 164		12.101	5.932	1.00 27.54	A
	MOTA	778			A 164		12.281	4.983	1.00 28.79	A
	ATOM	779	ND2		A 164		11.024	6.704	1.00 27.13	A
55	ATOM	780	С		A 164		14.931	5.169	1.00 24.43	A
	ATOM	781	0		A 164		15.856	5.589	1.00 23.98	A
	MOTA	782	N		A 165		15.097	4.795	1.00 21.56	A
	MOTA	783	CA		A 165		16.414	4.836	1.00 24.39	A
	MOTA	784	С	GLY	A 165	34.191	17.043	6.181	1.00 23.62	Α

	ATOM	785	0	GLY A 16	65	34.380	16.352	7.177	1.00 23.26	A
	ATOM	786		GLU A 16		34.234	18.373	6.186	1.00 23.22	A
	ATOM	787	CA	GLU A 16		34.563	19.176	7.362	1.00 24.54	A
		788	CB	GLU A 16		35.055	20.558	6.913	1.00 25.04	A
-	ATOM					36.419	20.569	6.229	1.00 26.48	Α
5	MOTA	789	CG	GLU A 16				5.517	1.00 30.02	A
	MOTA	790	CD	GLU A 1		36.699	21.889			A
	MOTA	791		GLU A 1		36.081	22.906	5.889	1.00 29.33	
	MOTA	792	OE2	GLU A 1	66	37.544	21.916	4.596	1.00 30.48	A
	MOTA	793	С	GLU A 1		33.436	19.372	8.369	1.00 24.44	A
10	ATOM	794	0	GLU A 1	66	32.279	19.541	8.001	1.00 22.76	A
	MOTA	795	N	LEU A 1	67	33.791	19.370	9.649	1.00 22.95	A
	ATOM	796	CA	LEU A 1	67	32.813	19.581	10.707	1.00 22.26	A
	MOTA	797	CB	LEU A 1	67	33.497	19.481	12.073	1.00 22.32	A
	ATOM	798	CG	LEU A 1	67	32.706	19.923	13.306	1.00 22.04	A
15	MOTA	799		LEU A 1		31.454	19.074	13.463	1.00 19.66	A
13		800		LEU A 1		33.597	19.805	14.537	1.00 21.17	A
	ATOM		C	LEU A 1		32.193	20.971	10.529	1.00 23.49	A
	ATOM	801		LEU A 1		31.047	21.209	10.907	1.00 23.56	A
	MOTA	802	0			32.960	21.887	9.948	1.00 24.25	A
	MOTA	803	Ŋ	LEU A 1			23.245	9.722	1.00 26.64	A
20	MOTA	804	CA	LEU A 1		32.473		9.066	1.00 25.62	A
	MOTA	805	CB	LEU A 1		33.560	24.099		1.00 27.34	A
	MOTA	806	CG	LEU A 1		33.198	25.546	8.707	1.00 27.34	A
	ATOM	807		LEU A 1		32.718	26.296	9.946		A
	ATOM	808	CD2	LEU A 1		34.418	26.238	8.119	1.00 26.74	
25	MOTA	809	C	LEU A 1	.68	31.234	23.218	8.829	1.00 27.13	A
	ATOM	810	0	LEU A 1	.68	30.297	23.989	9.030	1.00 26.01	A
	MOTA	811	N	LYS A 1	.69	31.233	22.320	7.848	1.00 26.41	A
	ATOM	812	CA	LYS A 1	.69	30.106	22.210	6.934	1.00 27.70	A
	ATOM	813	CB	LYS A 1	.69	30.324	21.064	5.945	1.00 30.49	A
30	ATOM	814	CG	LYS A 1	.69	29.151	20.854	4.993	1.00 32.47	Α
50	ATOM	815	CD	LYS A 1	.69	29.407	19.728	3.998	1.00 35.98	A
	ATOM	816	CE	LYS A 1		29.462	18.372	4.683	1.00 38.53	Α
	ATOM	817	NZ	LYS A 1		29.622	17.263	3.702	1.00 41.00	A
	ATOM	818	C	LYS A 1		28.801	21.985	7.682	1.00 28.12	A
35	ATOM	819	Ö	LYS A 1		27.785	22.608	7.371	1.00 28.08	A
33		820	N	TYR A 1		28.826	21.094	8.668	1.00 26.53	A
	ATOM		CA	TYR A 1		27.624	20.791	9.434	1.00 26.95	Α
	MOTA	821	CB	TYR A 1		27.810	19.476	10.193	1.00 25.03	A
	ATOM	822		TYR A 1		27.898	18.300	9.251	1.00 26.65	A
4.0	MOTA	823	CG			26.745	17.661	8.790	1.00 28.27	A
40	ATOM	824		TYR A 1			16.642	7.839	1.00 26.85	A
	MOTA	825		TYR A 1	-	26.814 29.127	17.884	8.742	1.00 27.83	A
	MOTA	826	CD2				16.869	7.792	1.00 27.19	A
	MOTA	827	CE2			29.209	16.254	7.343	1.00 30.02	A
	MOTA	828	cz	TYR A		28.049				A
45	MOTA	829	ОН	TYR A			15.268	6.382		A
	ATOM	830	С	TYR A		27.229	21.918	10.376	1.00 27.59	A
	MOTA	831	0	TYR A		26.045	22.122	10.642	1.00 29.25	
	ATOM	832	N	ILE A :	171	28.208	22.660	10.882	1.00 28.16	A
	ATOM	833	CA	ILE A	171	27.883	23.770	11.763	1.00 29.03	A
50	ATOM	834	CB	ILE A	171	29.151	24.435	12.337	1.00 27.51	A
	ATOM	835	CG2	LE A		28.773	25.705	13.084	1.00 27.97	A
	ATOM	836		ILE A		29.872	23.458	13.272	1.00 26.70	A
	ATOM	837		ILE A		31.163	23.996	13.856	1.00 24.07	A
	MOTA	838	C	ILE A		27.094	24.796	10.944	1.00 31.41	A
55	MOTA	839		ILE A		26.088	25.335	11.407	1.00 31.69	A
"	MOTA	840		ARG A		27.546	25.047	9.719		A
	ATOM	841		ARG A		26.874	26.000	8.844	1.00 36.54	A
		842		ARG A		27.734	26.314	7.616	1.00 37.73	A
	ATOM			ARG A		29.057	27.011	7.912		A
	MOTA	843	CG	M(O A		_2				

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	MOTA	844			A 17		29.70		27.492	6.616		45.29	A
	MOTA	845	NE I	ARG .	A 17	2	31.03		28.070	6.812		48.51	A
	MOTA	846			A 17		31.33		29.059	7.658		51.53	A
	MOTA		NH1				30.3		29.593	8.406		53.75	A N
5	MOTA	848	NH2				32.5		29.526	7.748		51.21	A A
	ATOM	849			A 17		25.5		25.459	8.378		37.67	A
	MOTA	850			A 17		24.5		26.200	8.288		39.09	A
	MOTA	851			A 17		25.4		24.163	8.092		38.44 39.25	A
	MOTA	852			A 17		24.2		23.528	7.619		41.89	A
10	MOTA	853			A 17		24.5		22.061	7.272		45.52	A
	MOTA	854			A 17		23.2		21.298	6.830		49.60	A
	MOTA	855			A 17		23.5		19.808	6.653 5.469		52.63	A
	MOTA	856			A 17		24.4		19.530			54.61	A
	MOTA	857			A 17		23.8		19.894	4.160 8.595		39.30	A
15	MOTA	858			A 17		23.0		23.608	8.201		39.62	A
	MOTA	859			A 17		21.9		23.960	9.863		37.96	. A
	MOTA	860	N		A 17		23.3		23.282	10.833		37.36	A
	ATOM	861	-		A 17		22.2		23.314 21.998	11.652		37.44	A
	MOTA	862	СВ		A 17		22.1		20.802	10.709		38.37	A
20	MOTA	863			A 17		22.0		21.850	12.532		37.25	A
	MOTA	864			A 17		23.3 23.3		20.620	13.418		36.85	A
	MOTA	865			A 17		22.2		24.492	11.801		36.71	A
	MOTA	866	C		A 17		21.4		24.556	12.724		38.05	A
	MOTA	867	0		A 17		23.1		25.423	11.592		35.48	A
25	MOTA	868	N		A 17 A 17		23.2		26.585	12.462		35.29	A
	ATOM	. 869	CA		A 17		24.0		26.360	13.737		35.06	A
	MOTA	870	C		A 1		25.0		27.019	13.970	1.00	37.46	A
	ATOM	871	O N		A 1'		23.5		25.441	14.571		33.94	A
20	ATOM	872	CA		A 1		24.2		25.113	15.822	1.00	32.84	A
30	MOTA	873	CB		A 1'		23.9		26.155	16.901	1.00	33.54	A
	ATOM	874 875	OG		A 1		22.5		26.056	17.347	1.00	34.86	A
	ATOM ATOM	876	C		A 1		23.7		23.731	16.276		0 32.34	A
	MOTA	877	0		A 1		22.7		23.263	15.884		0 32.82	A
35	ATOM	878	N		A 1		24.6	509	23.085	17.103		0 29.39	A
22	ATOM	879	CA		A 1		24.3	313	21.743	17.597		0 27.20	A
	ATOM	880	CB		A 1		25.0	621	20.989	17.865		0 26.39	A
	ATOM	881	CG		A 1		26.3	372	20.585	16.622		0 26.18	A
	ATOM	882	CD1	PHE	A 1	77	26.	210	21.277	15.426		0 25.30	A
40	ATOM	883	CD2	PHE	A 1	77	27.	266	19.516	16.662		0 26.05	. A
	ATOM	884	CE1	PHE	A 1	77	26.	923	20.912	14.290		0 26.59	A
	MOTA	885	CE2	PHE	; A 1	77	27.	986	19.143	15.532		0 26.06	A A
	ATOM	886	CZ		: A 1		27.		19.841	14.343		0 25.42	A
	MOTA	887	C	PHE	: A 1	.77	23.	500	21.752	18.884		0 27.00 0 26.48	A
45	MOTA	888	0	PHE	: A 1	.77	23.		22.610	19.747			A.
	MOTA	88 <i>9</i>	И) A 1		22.		20.802	19.022		0 26.70 0 26.35	A
	MOTA	890	CA		P A 1			816	20.729	20.260		0 29.90	A
	ATOM	891	CB		P A 1		20.		19.773	20.142	_	0 32.28	A
	ATOM	892	CG		P A 1			020	18.372	19.720		0 35.21	A
50	MOTA	893			P A 1			157	17.949	20.014	_	0 34.79	A
	MOTA	894	OD2		P A 1			179	17.683	19.109		0 25.03	A
	MOTA	895	C	-	? A 1			810	20.228	21.31		0 21.24	A
	MOTA	896			P A 1			974	19.968	20.99		0 23.60	A
	MOTA	897			JA 1			361	20.083		_	0 25.18	A
55	MOTA	898			JAI			247	19.644 19.770			0 27.60	
	MOTA	899			JAJ			542 324	19.776			0 32.58	
	MOTA	900			JAI							00 35.82	
	MOTA	901			U A :			. 997 . 825	20.224			00 35.95	A
	MOTA	902	OE:	اللكى ا	U A :	. 17	21.		20,224	, ~,			

	ATOM	903	OE2	GLU A	179	23.912	19.984	28.291	1.00 38.19	Α
	ATOM	904	C	GLU A	179	23.808	18.235	23.450	1.00 24.08	A
	MOTA	905	0	GLU A	179	24.977	17.989	23.756	1.00 22.79	A
	MOTA	906	N	THR A	180	22.983	17.316	22.961	1.00 23.36	A
. 5	ATOM	907	CA	THR A	180	23.412	15.935	22.761	1.00 22.15	A
	ATOM	908	CB	THR A	180	22.224	15.054	22.320	1.00 23.77	A
	ATOM	909	OG1	THR A	180	21.222	15.075	23.341	1.00 26.37	A
	ATOM	910	CG2	THR A	180	22.670	13.616	22.088	1.00 22.66	A
	ATOM	911	C	THR A		24.533	15.830	21.724	1.00 22.01	A
10	ATOM	912	ō	THR A		25.533	15.141	21.944	1.00 19.87	A
	ATOM	913	N	CYS A		24.365	16.511	20.596	1.00 21.21	A
	ATOM	914	CA	CYS A		25.372	16.480	19.541	1.00 22.22	A
	ATOM	915	CB	CYS P		24.800	17.065	18.250	1.00 24.62	, A
	ATOM	916	SG	CYS F		23.435	16.080	17.560	1.00 29.50	A
15	ATOM	917	C	CYS F		26.633	17.232	19.954	1.00 23.07	A
15	ATOM	918	Ö	CYS A		27.746	16.827	19.608	1.00 23.95	A
	ATOM	919	N	THR A		26.463	18.325	20.695	1.00 22.76	A
	ATOM	920	CA	THR A		27.606	19.103	21.161	1.00 21.49	. A
	ATOM	921	CB		A 182	27.167	20.346	21.978	1.00 21.37	A
20		922	OG1		A 182	26.459	21.262	21.134	1.00 22.50	Α
20	ATOM	923	CG2		A 182	28.379	21.046	22.565	1.00 18.36	A
	ATOM	924	C		A 182	28.454	18.215	22.071	1.00 21.48	. A
	ATOM	925	Ö	THR		29.669	18.090	21.894	1.00 19.95	A
	ATOM	926	И		A 183	27.798	17.602	23.050	1.00 18.97	A
25	ATOM	920 927	CA		A 183	28.468	16.723	23.996	1.00 19.39	A
25	ATOM	928	CB		A 183	27.455	16.140	24.984	1.00 19.46	Α
	ATOM	929	CG		A 183	28.030	15.062	25.887	1.00 18.77	A
	ATOM	930	CD		A 183	27.021	14.571	26.925	1.00 21.19	A
	MOTA	931	NE		A 183	26.605	15.642	27.824	1.00 19.46	A
20	ATOM	931	CZ		A 183	25.496	16.362	27.679	1.00 20.45	A
30	ATOM		NH1			24.672	16.123	26.666	1.00 19.81	A
	MOTA	933	NH2		A 183	25.224	17.338	28.539	1.00 17.11	A
	MOTA	934	C		A 183	29.206	15.577	23.302	1.00 20.02	A
	MOTA	935 936	Ö		A 183	30.383	15.333	23.573	1.00 19.97	A
25	MOTA	937	Ŋ		A 184	28.520	14.871	22.409	1.00 19.24	A
35	MOTA	938	CA		A 184	29.144	13.746	21.722	1.00 18.04	Α
	ATOM		CB		A 184	28.158	13.078	20.764	1.00 21.05	· А
	MOTA	939	CG		A 184	28.719	11.857	20.098	1.00 22.67	Α.
	MOTA	940		L PHE		28.717	10.630	20.754	1.00 22.97	A
40	MOTA	941		2 PHE		29.317	11.949	18.850	1.00 19.97	Α
40	MOTA	942		l PHE		29.308	9.510	20.176	1.00 23.53	· A
	ATOM	943		2 PHE		29.915	10.833	18.263	1.00 24.11	A
	MOTA	944	CZ		A 184	29.910	9.613	18.928	1.00 22.97	A
	MOTA	945	C		A 184	30.403	14.127	20.941	1.00 17.99	A
	MOTA	946	_		A 184	31.461	13.531	21.130	1.00 18.89	Α
45	MOTA	947	O		A 185	30.292	15.110	20.056	1.00 15.73	A
	MOTA	948	N		A 185	. 31.443	15.519	19.265	1.00 15.72	· A
	ATOM	949	CA			30.992	16.413	18.111	1.00 17.33	A
	MOTA	950	CB		A 185	30.364		17.015	1.00 19.37	A
	MOTA	951	CG	1 TYR	A 185	31.159		16.168	1.00 16.53	A
50	ATOM	952		1 TYR		30.590		15.232	1.00 18.12	A
	ATOM	953		2 TYR		28.976		16.892	1.00 18.18	A
	ATOM	954			A 185	28.398		15.956		A
	MOTA	955	CE		A 185	29.211			40 44	A
	MOTA	956	CZ OH		A 185	28.650				A
. 55	ATOM	957	C		A 185	32.544				A
	ATOM	958			A 185	33.720			45 60	A
	MOTA	959			A 186	32.176				A
	ATOM	960				33.184				Α
	ATOM	961	CA	TUK	A 186	33.104	27.504	21.221		

				•						
١	⊼ TTOM	962	СВ	THR A 186		32.559	18.403	23.094	1.00 16.62	A
	MOTA	963		THR A 186		31.866	19.503	22.481	1.00 14.79	A
	MOTA		CG2			33.656	18.953	24.019	1.00 14.68	A
	ATOM	964		•		33.954	16.375	22.680	1.00 15.59	A
_	MOTA	965	C	THR A 186			16.443	22.823	1.00 13.77	A
5	MOTA	966	0	THR A 186		35.176		23.097	1.00 14.06	A
	MOTA	967	N	ALA A 187		33.234	15.333		1.00 14.74	A
	MOTA	968	CA	ALA A 187		33.869	14.196	23.757	1.00 14.74	A
	MOTA	969	CB	ALA A 187		32.810	13.195	24.224	•	
	MOTA	970	C	ALA A 187		34.875	13.509	22.821	1.00 14.41	- A
10	ATOM	971	0	ALA A 187		35.972	13.136	23.247	1.00 15.61	A
	MOTA	972	N	GLU A 188		34.516	13.340	21.549	1.00 14.01	A
	MOTA	973	CA	GLU A 188		35.443	12.704	20.615	1.00 13.50	A
	ATOM	974	CB	GLU A 188		34.782	12.449	19.251	1.00 12.85	A
	ATOM	975	CG	GLU A 188		33.622	11.454	19.282	1.00 12.71	A
15	MOTA	976	CD	GLU A 188		33.464	10.685	17.979	1.00 15.01	A
	ATOM	977	OE1	GLU A 188		33.687	11.275	16.899	1.00 13.21	A
	ATOM	978	OE2	GLU A 188		33.110	9.484	18.031	1.00 17.69	A
	MOTA	979	C	GLU A 188		36.682	13.582	20.436	1.00 13.34	A
	ATOM .	980	ō	GLU A 188		37.803	13.085	20.408	1.00 14.69	A
20	ATOM	981	N	ILE A 189		36.486	14.893	20.326	1.00 13.52	A
20		982	CA	ILE A 189		37.627	15.787	20.159	1.00 13.35	A
	MOTA			ILE A 189		37.169	17.247	19.939	1.00 13.95	A
	MOTA	983	CB	ILE A 189		38.381	18.165	19.822	1.00 12.47	A
	MOTA	984				36.302	17.332	18.671	1.00 13.44	A
	MOTA	985		ILE A 189		35.588	18.664	18.491	1.00 14.29	A
25	MOTA	986		ILE A 189			15.702	21.394	1.00 14.63	Α
	MOTA	987	C	ILE A 189		38.530		21.271	1.00 12.97	A
	MOTA	988	0	ILE A 189		39.753	15.595	22.582	1.00 14.35	A
	MOTA	989	И	VAL A 190		37.927	15.751		1.00 14.33	Ā
	ATOM	990	CA	VAL A 190		38.684	15.655	23.832	•	A
30	MOTA	991	CB	VAL A 190		37.743	15.690	25.061	1.00 14.28	
	MOTA	992	CG1	VAL A 190		38.509	15.267	26.326	1.00 15.08	A
	MOTA	993	CG2	VAL A 190		37.160	17.082	25.233	1.00 12.08	A
	MOTA	994	С	VAL A 190		39.468	14,338	23.859	1.00 14.61	A
	ATOM	995	0	VAL A 190		40.634	14.304	24.250	1.00 13.72	A
35	MOTA	996	N	SER A 191		38.825	13.254	23.432	1.00 15.26	A
	ATOM	997	CA	SER A 191	•	39.478	11.943	23.421	1.00 16.81	A
	ATOM	998	CB	SER A 191		38.470	10.857	23.041	1.00 16.14	A
	ATOM	999	OG	SER A 191		39.018	9.569	23.238	1.00 16.94	A
	ATOM	1000	C	SER A 191		40.649	11.928	22.441	1.00 16.58	A
40	ATOM	1001	ō	SER A 191		41.697	11.335	22.713	1.00 13.96	Α
40		1002	N	ALA A 192		40.468	12.586	21.300	1.00 15.26	A
	MOTA		CA	ALA A 192		41.518	12.645	20.292	1.00 14.37	A
	MOTA	1003	CB	ALA A 192		40.989	13.296	19.016	1.00 14.43	Α
	MOTA	1004				42.695	13.440	20.845	1.00 16.46	A
	MOTA	1005	_			43.851	13.038	20.697	1.00 17.96	A
45	MOTA	1006	0	ALA A 192			14.563	21.496	1.00 15.02	· A
	MOTA	1007	N	LEU A 193		42.401	15.392	22.067	1.00 15.42	A
	ATOM	1008	CA	LEU A 193		43.459		22.600	1.00 12.88	A
	MOTA	1009	CB	LEU A 193		42.884	16.712		1.00 15.97	A
-	ATOM	1010	CG			42.445	17.721	21.525		A
50	ATOM	1011		1 LEU A 193		41.869	18.979		1.00 13.97	A
	MOTA	1012	CD:	2 LEU A 193		43.642	18.088	20.655	1.00 14.58	
	MOTA	1013	С	LEU A 193		44.211	14.659		1.00 14.49	A
	ATOM	1014	0	LEU A 193		45.427	14.813		1.00 16.56	. A
	ATOM	1015	N	GLU A 194		43.500	13.870		1.00 13.96	A
55	ATOM	1016	CA	GĽU A 194		44.179	13,123		1.00 14.08	A
	ATOM	1017				43.190	12.295			A
	ATOM	1018				43.882	11.301			A
	MOTA	1019				42.924		27.730	1.00 19.59	A
	MOTA	1020		1 GLU A 194		41.809		27.295	1.00 19.25	A
	ALOM					•				

	ATOM	1021	OE2 GL	JA	194	43	.302	10.380	28.906		20.20	A
	ATOM	1022	-	JA		45		12.199	24.386		13.57	A
	ATOM	1023	O GLI	JA	194	46	.337	12.093	24.847		14.23	A
	ATOM	1024	N TY	R A	195	44		11.544	23.301		14.89	A
5	MOTA	1025		A S				10.642	22.618		16.58	A
	MOTA	1026	CB TY	R A	195	45	.030	9.910	21.488		17.29	A
	ATOM	1027		R A			.956	9.058	20.649		17.92	A A
	MOTA	1028	CD1 TY	R A	195		.347	7.788	21.077		17.96	A
	MOTA	1029	CE1 TY	R A	195		.203	6.996	20.304		19.77	A
10	ATOM	1030	CD2 TY	R A	195		.445	9.524	19.428		16.67	A
	MOTA	1031	CE2 TY	R A	195		.299	8.744	18.650		18.51 20.24	A
	ATOM	1032	CZ TY	R A	195	47	.671	7.481	19.094			A
	ATOM	1033	OH TY	R A	195		.506	6.705	18.325		21.89	A
	MOTA	1034	C TY	R A	195		.917	11.419	22.035		16.98	A
15	MOTA	1035	O TY	R A	195	48	.081	11.047	22.203		14.61	A
	MOTA	1036	N LE	U A	196	46	.599	12.507	21.347		16.30	A
	MOTA	1037	CA LE	U A	196	47	.619	13.328	20.720		18.15	A
	MOTA	1038	CB LE	UA	196	46	.969	14.502	19.982		18.59	A
	MOTA	1039	CG LE	U A	196	47	.834	15.203	18.935		22.51	
20	ATOM	1040	CD1 LE	U A	196	48	.222	14.206	17.841		20.94	A
	ATOM	1041	CD2 LE	U A	196	47	.060	16.375	18.338		22.98	A
	ATOM	1042	C LE	U A	196	48	.592	13.844	21.763		17.75	A
	ATOM	1043	O LE	υA	196	49	.801	13.644	21.649		18.33	A
	ATOM	1044	N HI	SA	197	. 48	3.064	14.495	22.792		17.12	A
25	MOTA	1045	CA H	SA	197-	48	3.913	15.042	23.842		18.47	A
20	ATOM	1046		SA	197	48	3.069	15.866	24.817		15.90	A
	ATOM	1047			197	47	7.571	17.152	24.231		19.15	A
	ATOM	1048	CD2 H			47	7.830	17.745	23.038		18.22	A
	ATOM	1049	ND1 H			46	5.704	17.992	24.897		17.47	A
30	ATOM	1050	CE1 H			46	5.450	19.047	24.139		19.74	A
50	ATOM	1051	NE2 H			47	7.119	18.921	23.007		15.69	A
	ATOM	1052			197	4.9	9.696	13.958	24.572		19.40	A
	ATOM	1053			197	50	0.823	14.192	25.021		19.42	A
	ATOM	1054			198	4 :	9.106	12.770	24.679		18.59	A
35	ATOM	1055		Y A	198	4	9.793	11.675	25.339		0 19.60	A
75	ATOM	1056			198	5	1.075	11.307	24.612		0 21.86	A
	ATOM	1057			198	5	1.963	10.682	25.186		0 23.09	A
	ATOM	1058			199	5.	1.174	11.687	23.341		0 22.81	A
	ATOM	1059			199	5	2.368	11.401	22.549	_	0 24.43	A
40	ATOM	1060			199	5	1.990	10.905	21.154		0 26.00	A
	ATOM	1061			199	5	1.378	9.520	21.133		0 30.98	A
	ATOM	1062			199	5	1.291	9.002	19.708		0 36.85	A
	ATOM	1063		YS A	199	5	0.832	7.559	19.682		0 40.37	A
	ATOM	1064			199	· 5	1.646	6.691	20.581		0 43.48	A
45	ATOM	1065			199		3.253	12.631	22.414		0 23.88	A
7,7	ATOM	1066			199	5	4.144	12.669			0 24.97	A
	ATOM	1067			200	5	2.997	13.638			0 24.00	A
	ATOM	1068			1 200	5	3.790	14.853			0 22.12	A
	ATOM	1069			200	5	3.665	15.632			0 22.14	A
50	MOTA	1070			A 200	5	4.632	16.231			0 22.41	A
50	ATOM	1071	-		A 201	5	2.475	15.630			0 20.00	A
	ATOM	1072			A 201	5	2.252	16.355	20.080		0 18.93	A
	MOTA	1073			A 201		1.784	15.414	18.955	1.0	0 19.70	A
	MOTA	1074			A 201	5	51.414	16.226			0 20.12	
55	ATOM	1075			A 201		52.880	14.395			0 20.03	
در	MOTA	1076			A 201	5	52.408	13.258		5 1.0	0 22.75	A
	MOTA	1077			A 201		51.193				0 19.87	A
	ATOM	1078			A 201		50.121	17.161		7 1.	00 20.08	A
	MOTA	1079			A 202		51.508		19.81	5 1.	00 19.94	A
	MION	1075										

	ATOM	1080	CA	ILE A 202		50.601	19.772	19.891	1.00 20.45	A
	MOTA	1081	CB	ILE A 202		51.352	21.040	20.356	1.00 22.21	A
	MOTA	1082	CG2	ILE A 202		50.381	22.220	20.470	1.00 22.67	A
	MOTA	1083	CG1	ILE A 202		52.033	20.775	21.700	1.00 24.19	Α
5	ATOM	1084	CD1	ILE A 202		52.914	21.920	22.169	1.00 25.39	Α
	MOTA	1085	C	ILE A 202		50.105	19.999	18.464	1.00 20.71	. A
	ATOM	1086	0	ILE A 202		50.910	20.067	17.538	1.00 19.48	A
	MOTA	1087	N	HIS A 203		48.795	20.108	18.270	1.00 18.65	A
	MOTA	1088	CA	HIS A 203		48.280	20.319	16.919	1.00 18.02	A
10	MOTA	1089	CB	HIS A 203		46.775	20.057	16.874	1.00 16.31	A
	MOTA	1090	CG	HIS A 203		46.199	20.136	15.495	1.00 18.36	A
	MOTA	1091	CD2	HIS A 203		46.043	21.186	14.655	1.00 16.42	A
	MOTA	1092		HIS A 203		45.759	19.026	14.806	1.00 19.50	A
•	ATOM	1093	CE1	HIS A 203		45.359	19.389	13.600	1.00 17.64	A
15	MOTA	1094	NE2	HIS A 203		45.522	20.694	13.483	1.00 20.87	A
	MOTA	1095	С	HIS A 203		48.589	21.738	16.405	1.00 18.92	A
	ATOM	1096	0	HIS A 203		49.073	21.906	15.282	1.00 16.21	A
	ATOM	1097	N	ARG A 204		48.301	22.744	17.232	1.00 18.60	. A
•	MOTA	1098	CA	ARG A 204		48.552	24.157	16.914	1.00 19.81	, A
20	ATOM	1099	CB	ARG A 204		49.998	24.365	16.458	1.00 21.61	A
	ATOM	1100	CG	ARG A 204		51.024	24.137	17.550	1.00 23.82	A
	ATOM	1101	CD	ARG A 204		52.323	24.870	17.252	1.00 27.62	A
	ATOM	1102	NE	ARG A 204		52.932	24.449	15.994	1.00 29.43	A
	ATOM	1103	CZ	ARG A 204		54.125	24.861	15.572	1.00 33.10	A
25	ATOM	1104	NHl	ARG A 204		54.835	25.706	16.311	1.00 32.12	A
	ATOM	1105	NH2	ARG A 204		54.614	24.426	14.418	1.00 30.25	A
	MOTA	1106	C	ARG A 204		47.624	24.830	15.905	1.00 20.03	A
	MOTA	1107	0	ARG A 204		47.711	26.038	15.698	1.00 20.88	A
•	MOTA	1108	N	ASP A 205		46.755	24.071	15.255	1.00 18.96	A
30	ATOM	1109	CA	ASP A 205		45.828	24.692	14.325	1.00 17.90	A
50	ATOM	1110	CB	ASP A 205		46.418	24.741	12.914	1.00 18.95	A
	ATOM	1111	CG	ASP A 205		45.655	25.688	12.008	1.00 20.36	A
	ATOM	1112	OD1	ASP A 205		44.939	26.560	12.545	1.00 20.35	A
	ATOM	1113	OD2	ASP A 205		45.772	25.573	10.771	1.00 22.49	A
35	ATOM	1114	C	ASP A 205		44.500	23.956	14.328	1.00 19.60	A
	ATOM	1115	0	ASP A 205		43.876	23.751	13.287	1.00 21.53	A
	MOTA	1116	N.	LEU A 206		44.063	23.569	15.521	1.00 18.53	A
	ATOM	1117	CA	LEU A 206		42.813	22.851	15.667	1.00 19.18	A A
	MOTA	1118	CB	LEU A 206		42.693	22.295	17.087	1.00 18.94	
40	ATOM	1119	CG	LEU A 206		41.511	21.358	17.346	1.00 23.10	A
	ATOM	1120	CD1	L LEU A 206		41.615	20.142	16.436	1.00 23.01	A A
	ATOM	1121	CD2	LEU A 206		41.504	20.933	18.808	1.00 22.97	A
	ATOM	1122	C	LEU A 206		41.639	23.772	15.361	1.00 19.05	A
	ATOM	1123	0	LEU A 206		41.556	24.880	15.886	1.00 19.25	A A
45	MOTA	1124	N	LYS A 207		40.740	23.307	14.500	1.00 17.54	A
	ATOM	1125	CA	LYS A 207		39.564	24.081	14.110	1.00 18.60	A
	ATOM	1126	CB	LYS A 207		39.980	25.248	13.196	1.00 18.98	A
	MOTA	1127	CG	LYS A 207		40.786	24.817	11.982	1.00 18.20	A
	MOTA	1128	CD	LYS A 207		41.246	26.000	11.139	1.00 21.42	A
50	MOTA	1129	CE	LYS A 207		42.223	25.537	10.062	1.00 23.21	A
	MOTA	1130	NZ	LYS A 207		42.561	26.604	9.084	1.00 29.61 1.00 18.18	A
	MOTA	1131	C	LYS A 207		38.566	23.181	13.388	1.00 18.10	A
	MOTA	1132	0	LYS A 207		38.921	22.100	12.915		A
	MOTA	1133	N	PRO A 208		37.298	23.614	13.293		A
55	MOTA	1134	CD			36.713	24.833	13.882		A
	MOTA	1135	CA		-	36.272	22.814	12.616		A
	MOTA	1136	CB			35.063	23.742	12.608		A
	MOTA	1137	CG			35.231	24.509	13.891		A
	MOTA	1138	С	PRO A 208		36.674	22.372	11.209	1.00 21.04	2.7

		1							
	ATOM	1139	0	PRO A 208	36.20			1.00 21.19	Α
	MOTA	1140	N	GLU A 209	37.4			1.00 21.69	A
	ATOM	1141	CA	GLU A 209	37.9			1.00 22.64	A
	ATOM	1142	CB	GLU A 209				1.00 23.65	A
5	MOTA	1143	CG	GLU A 209	39.2			1.00 27.24	A
	MOTA	1144	CD	GLU A 209				1.00 29.40	A
	MOTA	1145	OE1	GLU A 209			•	1.00 29.68	A
	MOTA	1146	OE2	GLU A 209				1.00 30.07	A
	MOTA	1147	C	GLU A 209				1.00 22.28	A
10	MOTA	1148	0	GLU A 209				1.00 21.36	A
	MOTA	1149	N	ASN A 210				1.00 19.90	A
	ATOM	1150	CA	ASN A 210				1.00 19.44	A
	ATOM	1151	CB	ASN A 210				1.00 20.07	A
	MOTA	1152	CG	ASN A 21		•		1.00 25.77	A
15	MOTA	1153		ASN A'21				1.00 26.73	A
	MOTA	1154	ND2	ASN A 21				1.00 25.15	A
	MOTA	1155	С	ASN A 21				1.00 18.63	A
	MOTA	1156	0	ASN A 21				1.00 18.29	A
	MOTA	1157	N	ILE A 21				1.00 16.31	A
20	MOTA	1158	CA	ILE A 21				1.00 15.49	A
	MOTA	1159	CB	ILE A 21				1.00 15.40	A
	MOTA	1160		ILE A 21				1.00 14.59	A
	ATOM	1161		ILE A 21				1.00 15.91	A A
	MOTA	1162	CD1	ILE A 21				1.00 15.98	
25	MOTA	1163	C	ILE A 21				1.00 17.26	A
	MOTA	1164	0	ILE A 21				1.00 18.16	. A A
	MOTA	1165	N	LEU A 21				1.00 15.97	A
	MOTA	1166	CA	LEU A 21				1.00 17.08	
	MOTA	1167	CB	LEU A 21					A
30	MOTA	1168	CG	LEU A 21				1.00 18.92	A
	MOTA	1169		LEU A 21				1.00 22.09	A
	MOTA	1170	CD2	LEU A 21				1.00 19.91	A
	MOTA	1171	С	LEU A 21				1.00 18.35	A
	MOTA	1172	0	LEU A 21				1.00 19.39 1.00 17.84	A
35	MOTA	1173	И	LEU A 21			_	1.00 17.84	A
	MOTA	1174	CA	LEU A 21				1.00 19.94	A
	ATOM	1175	CB	LEU A 21	_			1.00 20.84	A
	ATOM	1176	CG	LEU A 21				1.00 20.31	A
	ATOM	1177		LEU A 21			_	1.00 23.93	A
40	ATOM	1178		LEU A 21				1.00 20.98	A
	ATOM	1179	. C	LEU A 21					A
	ATOM	1180	0	LEU A 21					A
	ATOM	1181	N	ASN A 21					A
	MOTA	1182	CA	ASN A 21					
45	MOTA	1183	CB	ASN A 21					A
	MOTA	1184	CG	ASN A 21					A
	MOTA	1185		ASN A 21		•			A
	MOTA	1186		ASN A 23					A
	MOTA	1187	C	ASN A 21					A
50	MOTA	1188	0	ASN A 21					A
	MOTA	1189	N	GLU A 21					A
	MOTA	1190	CA	GLU A 21					A
	ATOM	1191	CB	GLU A 21					A
	MOTA	1192	CG	GLU A 2					A
55	MOTA	1193	CD	GLU A 2					A
	MOTA	1194		GLU A 2					A
	MOTA	1195		GLU A 2					
	MOTA	1196	C	GLU A 2			-		A
	ATOM	1197	0	GLU A 2	15 28.	211 /·/t	,, ,,,,,,		

	ATOM	1198	N	ASP A	216	3 (737	7.287	8.752	1.00 26.77	A
	MOTA	1199	CA	ASP A	216	29	9.914	6.953	9.917	1.00 27.28	A
	MOTA	1200	CB	ASP A	216	3 (0.538	5.795	10.696	1.00 31.27	A
	MOTA	1201	CG	ASP A	216	3 (390	4.466	9.979	1.00 37.61	Α
5	MOTA	1202	OD1	ASP A	216	2.9	9.274	4.170	9.499	1.00 39.45	A
	ATOM	1203	OD2	ASP A	216	3	1.382	3.710	9.902	1.00 41.84	Α.
	ATOM ·	1204	С	ASP A	216	25	9.697	8.135	10.862	1.00 26.37	A
	ATOM	1205	0	ASP A	216	25	9.136	7.984	11.950	1.00 25.73	A
	MOTA	1206	N	MET A	217	3 (0.156	9.306	10.441	1.00 23.02	A
10	MOTA	1207	CA	MET A	217	3 (0.015	10.527	11.218	1.00 21.83	A
	MOTA	1208	CB	MET A	217	21	8.537	10.789	11.517	1.00 23.24	A
	MOTA	1209	CG	MET A			7.742	11.186	10.274	1.00 22.98	A
	MOTA	1210	SD	MET A			8.464	12.616	9.430	1.00 27.57	A
	MOTA	1211	CE	MET A			7.679	13.974	10.332	1.00 26.68	A
15	ATOM	1212	С	MET A			0.844	10.618	12.502	1.00 21.51	A
	MOTA	1213	0	MET A			0.474	11.323	13.440	1.00 18.62	A
	ATOM	1214	N	HIS A			1.957	9.892	12.544	1.00 20.10	A
	MOTA	1215	CA	HIS A			2.873	9.964	13.678	1.00 19.86	A
	MOTA	1216	CB	HIS A			3.482	8.594	13.977	1.00 20.21	A
20	MOTA	1217	CG	HIS A			2.551	7.667	14.698	1.00 22.40	A
	MOTA	1218		HIS A			1.910	6.547	14.287	1.00 21.27	A
	MOTA	1219		HIS A			2.177	7.863	16.011	1.00 19.59	A
	MOTA	1220		HIS A			1.348	6.902	16.379	1.00 21.88	A
	ATOM	1221	NE2	HIS A			1.168	6.091	15.351	1.00 22.08	A
25	MOTA	1222	C	HIS A			3.947	10.921	13.172	1.00 19.10	A A
	MOTA	1223	0	HIS A			4.170	11.004	11.965	1.00 20.31	
	ATOM	1224	И	ILE A			4.617	11.638	14.067	1.00 17.21	A A
	MOTA	1225	CA	ILE A		-	5.628	12.586	13.618	1.00 15.26	A
	MOTA	1226	CB.	ILE A			5.987	13.614	14.716	1.00 15.38 1.00 14.58	A
30	MOTA	1227		ILE A			4.722	14.305	15.221	1.00 14.36	A
	ATOM	1228		ILE A			6.734	12.919	15.864	1.00 14.46	A
	ATOM	1229		ILE A			7.279	13.885	16.911	1.00 15.74	A
	MOTA	1230	C	ILE A			6.929	11.944	13.161	1.00 15.21	A
	MOTA .	1231	0	ILE A			7.238	10.799	13.500	1.00 15.62	A
35	MOTA	1232	N	GLN A			7.677	12.711	12.378 11.876	1.00 13.02	A
	MOTA	1233	CA	GLN A			8.980	12.316		1.00 20.00	A
	MOTA	1234	CB	GLN A			8.872	11.595	10.525 10.659	1.00 26.97	A
	MOTA	1235	CG	GLN A			8.463	10.129 9.343	9.372	1.00 20.57	A
	MOTA	1236	CD	GLN A			8.648	9.590	8.373	1.00 23.33	A
40	MOTA	1237		GLN A			7.968	8.393	9.389	1.00 30.47	A
	MOTA	1238	NE2				9.578	13.610	11.735	1.00 17.00	A
	ATOM	1239	C	GLN A			19.757 19.609	14.339	10.751	1.00 18.27	A
	ATOM	1240	0	GLN A			10.566	13.906	12.746	1.00 14.34	A
	ATOM	1241	N	ILE A	7 221		11.361	15.120	12.753	1.00 14.46	A
45	ATOM	1242	CA	ILE A			1.867	15.126	14.175	1.00 12.30	A
	ATOM	1243	CB		A 221		12.764	16.656	14.167	1.00 14.78	A
	ATOM	1244		ILE A			10.660	15.613	15.102	1.00 13.92	A
	MOTA	1245		ILE A			11.003	15.901	16.543	1.00 15.06	A
	ATOM	1246		L ILE A			12.536	14.996	11.783	1.00 15.44	A
50	ATOM	1247	C		A 221 A 221		13.106	13.915	11.613	1.00 13.93	A
	ATOM	1248	0		A 221		12.877	16.101	11.127	1.00 15.36	A
	ATOM	1249	N				13.980	16.098	10.174	1.00 17.52	A
	MOTA	1250	CA		A 222 A 222		43.470	15.836	8.750	1.00 19.92	A
<i></i>	ATOM	1251	CB	THR A			44.587	15.637	7.875	1.00 18.78	A
55	ATOM	1252		THR A			42.630	17.018	8.257		A
	ATOM	1253			A 222		44.735	17.428	10.192		A
	MOTA	1254	C		A 222		44.509		11.084		A
	MOTA	1255	О М		A 223		45.630		9.216		A
	MOTA	1256	N	ADF .	223					=:	

	ATOM	1257	CA	ASP A	223	46.440	18.825	9.069	1.00 20.12	A
	MOTA	1258	CB	ASP A	223	45.532	20.065	9.108	1.00 23.51	A
	MOTA	1259	CG	ASP A	223	46.248	21.335	8.670	1.00 27.09	Α
	MOTA	1260	OD1	ASP A	223	47.283	21.227	7.975	1.00 26.28	A
5	ATOM	1261	OD2	ASP A	223	45.765	22.438	9.009	1.00 26.15	A
	MOTA	1262	C	ASP A	223	47.516	18.913	10.150	1.00 21.73	A
	MOTA	1263	0	ASP A	223	47.439	19.751	11.055	1.00 22.76	A
×	ATOM	1264	N	PHE A	224	48.535	18.063	10.027	1.00 20.75	A
	ATOM	1265	CA	PHE A		49.611	17.988	11.009	1.00 20.11	A
10	ATOM	1266	CB	PHE A		49.805	16.527	11.424	1.00 20.62	A
	MOTA	1267	CG	PHE A		48.682	15.991	12.263	1.00 21.41	A
	MOTA	1268		PHE A		48.598	16.312	13.614	1.00 23.05	A
	MOTA	1269		PHE A		47.681	15.212	11.693	1.00 22.27	A
	MOTA	1270		PHE A		47.528	15.868	14.389	1.00 23.30	A
15	MOTA	1271				46.606	14.763	12.457	1.00 21.11	A
	ATOM	1272	CZ	PHE A		46.530	15.093	13.807	1.00 22.02	A
٠	MOTA	1273	C	PHE A		50.957	18.583	10.619	1.00 20.45	A A
	MOTA	1274	0	PHE A		51.905	18.547	11.407	1.00 20.73	. A
	MOTA	1275	и.	GLY A		51.049	19.125	9.412 8.981	1.00 22.02 1.00 22.66	A
20	MOTA	1276	CA	GLY A		52.301	19.713		1.00 22.88	A
	MOTA	1277	C	GLY A		52.742	20.822	9.920 10.122	1.00 24.53	A
	MOTA	1278	0	GLY A		53.939		10.122	1.00 24.52	A
	MOTA	1279	N	THR A		51.779	21.524	11.416	1.00 25.30	A
	MOTA	1280	CA	THR A		52.106	22.613 23.829	11.410	1.00 23.10	A
25	MOTA	1281	CB	THR A		51.199	23.410	11.113	1.00 22.68	A
	ATOM	1282	OG1			49.831 51.571	24.490	9.834	1.00 25.00	A
	MOTA	1283	CG2	THR A		52.046	22.233	12.894	1.00 25.79	A
	MOTA	1284	C	THR A		52.019	23.100	13.768	1.00 24.54	. A
` 20	ATOM	1285	0	THR A		52.037	20.935	13.173	1.00 24.97	A
30	MOTA	1286	N	ALA A		52.004	20.475	14.550	1.00 25.49	A
	ATOM	1287	CA CB	ALA A		51.659	18.993	14.607	1.00 22.85	A
	MOTA	1288	С	ALA A		53.384	20.715	15.149	1.00 27.70	A
	ATOM ATÓM	1289 1290	0	ALA A		54.331	21.047	14.435	1.00 26.60	A
35	ATOM	1291	И	LYS A		53.491	20.558	16.461	1.00 28.53	A
33	ATOM	1292	CA	LYS A		54.760	20.745	17.149	1.00 32.12	A
	ATOM	1293	CB	LYS A		54.699	21.974	18.054	1.00 33.81	A
	ATOM	1294	CG	LYS A		56.007	22.294	18.765	1.00 41.23	A
	ATOM	1295	CD	LYS F		57.082	22.725	17.768	1.00 47.57	A
40	ATOM	1296	CE	LYS A		58.401	23.056	18.462	1.00 49.82	A
70	ATOM	1297	NZ	LYS A		59.459	23.425	17.480	1.00 51.49	A
	MOTA	1298	C	LYS A		55.019	19.504	17.985	1.00 33.25	A
	ATOM	1299	0	LYS 1		54.190	19.129	18.815	1.00 33.70	A
	MOTA	1300	N	VAL A	A 229	56.159	18.860	17.756	1.00 33.64	A
45	ATOM	1301	CA	VAL A	A 229	56.516	17.661	18.501	1.00 34.66	A
	ATOM	1302	CB	VAL A	A 229	57.248	16.646	17.609	1.00 33.50	A
	ATOM	1303	CG1	VAL A	A 229	57.619	15.419	18.415	1.00 32.34	A
	MOTA	1304	CG2	VAL A	A 229	56.370	16.264	16.436	1.00 34.25	A
	MOTA	1305	C	VAL A	A 229	57.420	18.035	19.668	1.00 37.57	A
50	MOTA	1306	0		A 229	58.581	18.392	19.474	1.00 35.91	A
	MOTA	1307	N		A 230	56.877	17.948	20.878	1.00 40.57	A
	ATOM	1308	CA		A 230	57.615	18.289	22.088	1.00 46.10	A A
	MOTA	1309	CB		A 230	56.654	18.417	23.270	1.00 44.71	A
	ATOM	1310	CG		A 230	55.627	19.545	23.207		A
55	MOTA	1311		L LEU		54.673	19.430	24.383		A
	MOTA	1312		LEU		56.340	20.885	23.214		A
	MOTA	1313	C		A 230	58.695	17.279	22.440		A
	MOTA	1314	0		A 230	58.603		22.089		A
	MOTA	1315	И	SER	A 231	59.717	17.756	23.145	1.00 22.01	••

	ATOM	1316	CA	SER	А	231	60.824	16.914	23.583	1.00 61.14	A
	ATOM	1317	СВ	SER	A	231	62.077	17.200	22.750	1.00 61.27	A
	ATOM	1318	OG	SER	Α	231	62.444	18.568	22.823	1.00 62.85	Α
	MOTA	1319	С	SER	A	231	61.124	17.126	25.071	1.00 64.65	A
5	ATOM	1320	0			231	61.392	16.164	25.794	1.00 65.70	Α
	ATOM	1321	N	PRO	Α	232	61.081	18.387	25.549	1.00 67.54	A
	MOTA	1322	CD	PRO	Α	232	60.854	19.651	24.823	1.00 68.60	A
	ATOM	1323	CA			232	61.358	18.655	26.966	1.00 68.74	Α
	ATOM	1324	CB	PRO	Α	232	61.109	20.158	27.086	1.00 68.83	A
10	ATOM	1325	CG	PRO	Α	232	61.505	20.666	25.737	1.00 68.96	A
	ATOM	1326	С	PRO	Α	232	60.460	17.846	27.899	1.00 69.17	Α
	ATOM	1327	o			232	59.335	17.494	27.541	1.00 69.94	A
	ATOM	1328	N	ALA	Α	237	57.424	23.198	27.637	1.00 80.06	A
	ATOM	1329	CA			237	56.783	23.047	26.335	1.00 79.29	A
15	ATOM	1330	CB			237	55.275	22.907	26.512	1.00 78.64	Α
10	ATOM	1331	C			237	57.092	24.239	25.433	1.00 79.07	A
	ATOM	1332	ō			237	56.250	25.113	25.249	1.00 79.47	A
	MOTA	1333	N			238	58.297	24.280	24.871	1.00 78.57	Α
	ATOM	1334	CA			238	58.683	25.383	23.992	1.00 78.50	A
20	ATOM	1335	CB			238	60.186	25.347	23.728	1.00 78.50	A
20	ATOM	1336	C			238	57.920	25.327	22.673	1.00 78.15	A
	ATOM	1337	Ö			238	57.243	24.341	22.375	1.00 77.96	Α
	MOTA	1338	N			239	58.027	26.393	21.887	1.00 77.28	A
	ATOM	1339	CA			239	57.338	26.452	20.603	1.00 76.27	, A
25	ATOM	1340	CB			239	55.849	26.489	20.827	1.00 76.61	A
23	ATOM	1341	C			239	57.766	27.667	19.793	1.00 75.38	A
	ATOM	1342	0			239	58.955	27.955	19.700	1.00 75.89	A
	ATOM	1343	N			240	56.781	28.357	19.214	1.00 73.95	A
	ATOM	1344	CA			240	56.967	29.553	18.389	1.00 71.07	A
30	ATOM	1345	CB			240	58.151	30.400	18.874	1.00 71.47	A
30	ATOM	1345	CG			240	59.459	30.055	18.174	1.00 72.06	A
	ATOM	1347		ASN			59.575	30.149	16.943	1.00 72.03	A
	ATOM	1347		ASN			60.470	29.665	18.964	1.00 71.91	A
	ATOM	1349	C			240	57.188	29.178	16.928	1.00 69.41	A
35		1350	0			240	57.480	28.024	16.624	1.00 70.09	A
22	MOTA	1351	N			241	57.055	30.165	16.038,	1.00 66.62	Α
	ATOM	1351	CA			241	57.246	30.013	14.585	1.00 63.94	· A
	ATOM	1352	CA			241	55.952	30.080	13.772	1.00 60.63	A
	ATOM	1354	0			241	55.840	30.880	12.845	1.00 61.29	A
40	ATOM		CB			241	57.979	28.704	14.246	1.00 65.23	A
40	MOTA	1355 1356	N			242	54.984	29.236	14.113	1.00 56.72	Α
	ATOM		CA			242	53.712	29.196	13.394	1.00 52.53	A
	ATOM	1357	CB			242	53.419	27.767	12.923	1.00 49.14	A
	ATOM	1358 1359	CG			242	52.040	27.590	12.354	1.00 47.38	Α
45	ATOM				_		51.731	28.067	11.085	1.00 47.69	A
45	ATOM	1360				242	51.038	26.975	13.102	1.00 45.45	A
•	ATOM	1361				242	50.445	27.937	10.565	1.00 46.75	Α
	ATOM	1362				242	49.751	26.840	12.594	1.00 45.41	A
	MOTA	1363				242	49.453	27.323	11.322	1.00 46.55	A
٠.	ATOM	1364	CZ			242	52.534	29.688	14.229	1.00 50.08	A
50	MOTA	1365	C			242	52.502	29.505	15.444	1.00 49.86	A
	MOTA	1366	0			242		30.305	13.557	1.00 47.67	A
	ATOM	1367	N			243	51.566 50.355	30.305	14.200	1.00 47.07	A
	MOTA	1368	CA			243	50.355	30.809	14.258	1.00 47.36	A
	MOTA	1369	CB			243	50.340 49.012	32.352	14.256	1.00 47.54	A
55	MOTA	1370				243	51.497		15.109	1.00 48.50	A
	MOTA	1371				243		32.842	13.389	1.00 44.12	· A
	MOTA	1372	С			243	49.150	30.342		1.00 44.12	A
	ATOM	1373	0			243	48.956	30.765	12.247	1.00 40.48	A
	MOTA	1374	N	GLY	P	244	48.348	29.467	13.985	1.00 40.40	**

	MOTA	1375	CA	GLY	Α	244	4	7.176	5	28.941	13.306	1.00 37.65	Α
	MOTA	1376	C	GLY	A	244	4	5.101	L	29.960	12.964	1.00 35.39	A
	ATOM	1377	0	GLY	A	244	4	5.313	3	31.168	13.065	1.00 35.92	A
	MOTA	1378	N	THR	Α	245	4	4.936	5	29.463	12.560	1.00 33.30	A
5	MOTA	1379	CA	THR	A	245	4	3.813	3	30.312	12.184	1.00 30.20	A
	MOTA	1380	CB	THR	Α	245	4	2.593		29.450	11.829	1.00 32.00	A
	ATOM	1381	OG1	THR	Α	245	4	2.952	2	28.573	10.755	1.00 32.81	A
	ATOM	1382	CG2	THR	Α	245	4	1.419	9	30.319	11.390	1.00 28.34	A
	ATOM	1383	C	THR	Α	245	4	3.476	6	31.296	13.296	1.00 27.96	A
10	ATOM	1384	0	THR	A	245	4	3.212	2	30.907	14.434	1.00 25.46	A
	ATOM	1385	N	ALA	A	246	4	3.486	6	32.576	12.938	1.00 25.22	A
	ATOM	1386	CA	ALA	Α	246	4	3.247	7	33.675	13.867	1.00 23.27	A
	ATOM	1387	СВ	ALA	Α	246	4	2.956	6	34.955	13.082	1.00 22.94	A
	MOTA	1388	C	ALA	Α	246	4	2.178	8	33.475	14.934	1.00 21.27	A
15	ATOM	1389	Ó			246	4	2.433	1	33.705	16.114	1.00 20.93	A
	ATOM	1390	N			247	4	0.988	8	33.047	14.536	1.00 19.67	A
	ATOM	1391	CA			247	3	9.91	1	32.886	15.504	1.00 20.17	A
	ATOM	1392	СВ			247	3	8.608	8	32.535	14.779	1.00 21.89	Α
	ATOM	1393	CG			247	3	8.522	2	33.076	13.355	1.00 26.18	A
20	ATOM	1394	CD			247		7.220		33.794	13.064	1.00 27.30	A
20	MOTA	1395		GLN				6.172		33.447	13.605	1.00 30.13	A
	ATOM	1396	NE2					7.27		34.792	12.189	1.00 28.70	A
	ATOM	1397	C			247		0.18		31.849	16.595	1.00 19.43	A
	ATOM	1398	ō			247		9.54		31.883	17.648	1.00 18.93	A
25	ATOM	1399	N			248		1.13		30.948	16.359	1.00 18.60	A
23	MOTA	1400	CA			248		1.44		29.896	17.329	1.00 19.20	A
	ATOM	1401	СВ			248		1.33		28.529	16.642	1.00 17.53	A
	ATOM	1402	CG			248		0.01		28.362	15.927	1.00 19.32	A
•	ATOM	1403		TYR				8.85		28.010	16.625	1.00 17.69	Α
30	ATOM	1404		TYR				7.61		27.976	15.990	1.00 18.18	A
30	ATOM	1405		TYR				9.89		28.664	14.569	1.00 16.87	·A
		1405		TYR				8.66		28.635	13.924	1.00 19.17	· A
	ATOM ATOM	1407	CZ			248		7.52		28.295	14.643	1.00 19.46	Α
		1408	OH			248		6.29		28.311	14.023	1.00 18.98	A
35	ATOM ATOM	1409	C			248		2.81		30.039	17.993	1.00 20.42	A
33		1410	o		•	248		3.20		29.191	18.792	1.00 19.19	A
	MOTA	1411	Ŋ			249		3.52		31.114	17.673	1.00 20.20	Α
	MOTA	1412	CA			249		4.84		31.343	18.251	1.00 20.91	A
	ATOM	1413	CB			249		5.54		32.532	17.570	1.00 21.18	· A
40	MOTA MOTA	1414		L VAL				6.82		32.896	18.317	1.00 22.45	A
40		1415		VAL				15.86		32.170	16.139	1.00 24.01	A
	MOTA		C			249		4.76		31.606	19.750	1.00 21.52	A
	MOTA	1416 1417	0			249		13.91		32.368	20.216	1.00 22.72	A
	MOTA	•	И			250		15.65		30.965	20.503	1.00 20.70	A
AF	ATOM	1418				250		15.69		31.133	21.951	1.00 21.65	· A
45	ATOM	1419	CA			250		16.37		29.919	22.613	1.00 22.02	. A
	ATOM	1420	CB			250		17.69		29.725	22.132	1.00 22.12	Α
	ATOM	1421						46.47		32.402	22.280	1.00 22.13	A
	ATOM	1422	C			250		47.33		32.828	21.511	1.00 22.77	Α
	ATOM	1423	0			251		46.18		33.029	23.425	1.00 22.23	A
50	ATOM	1424	N					45.16		32.684	24.433	1.00 22.97	Α
	ATOM	1425	CD			251		46.89		34.254	23.800	1.00 22.52	A
	MOTA	1426	CA			251		46.23		34.650	25.127		A
	ATOM	1427	CB			251		45.72		33.329	25.676		A
<i>-</i> -	ATOM	1428	CG			251		43.72 48.41		34.115	23.907		A
55	ATOM	1429	C					40.41 49.14		35.047	23.563		A
	ATOM	1430	0			251 252		49.14 48.90		32.966			· A
	ATOM	1431				252		50.34		32.772	24.500		A
	ATOM	1432								31.382	25.071		A
	ATOM	1433	CB	باداق	, f	252		50.67	13	21.202	23.0/1	1.00 00.00	

	ATOM	1434	CG	GLU	А	252	49.993	30.232	24.352	1.00 21.91	A
	ATOM	1435	CD	GLU			48.691		25.014	1.00 21.51	A
	ATOM	1436	OE1				47.989		25.550	1.00 21.46	A
	ATOM	1437	OE2				48.367		24.993	1.00 20.23	A
5	ATOM	1438	C	GLU			51.071		23.167	1.00 22.99	A
-	ATOM	1439	0	GLU			52.191		23.136	1.00 23.17	A
	ATOM	1440	И	LEU			50.441		22.064	1.00 23.00	A
	ATOM	1441	CA	LEU			51.068		20.758	1.00 25.62	A
	ATOM	1442	CB	LEU			50.277		19.669	1.00 26.75	A
10	ATOM	1443	CG	LEU			50.743		19.296	1.00 31.87	A
10	ATOM	1444		LEU			50.433		20.422	1.00 31.81	A
	ATOM	1445	CD2				50.044		18.015	1.00 31.86	A
	ATOM	1446	CDZ	LEU			51.201		20.371	1:00 31.00	A
		1447	0	LEU			52.107		19.626	1.00 27.09	A
15	ATOM								20.877	1.00 27.03	A
15	ATOM	1448	N	LEU			50.297		20.564	1.00 23.83	A
•	ATOM	1449	CA	LEU			50.297				
	ATOM	1450	СВ	LEU			48.858		20.564	1.00 25.84	A
	MOTA	1451	CG			254	47.882		19.621	1.00 24.69	
••	ATOM	1452		LEU			46.459		19.932	1.00 23.64	A
20	MOTA	1453		LEU			48.236		18.177	1.00 24.24	
	MOTA	1454	C			254	51.134		21.537	1.00 30.62	A
	MOTA	1455	0			254	51.633		21.187	1.00 32.35	
	MOTA	1456	и.	THR	A	255	51.292	_	22.758	1.00 32.47	
	MOTA	1457	CA	THR	Α	255	52.056		23.759	1.00 36.70	
25	ATOM	1458	CB	THR	Α	255	51.368	37.478	25.127	1.00 34.51	
	MOTA	1459	OG1	THR	Α	255	51.188	36.106	25.494	1.00 35.49	
	ATOM	1460	CG2	THR	Α	255	50.013	38.166	25.077	1.00 33.40	
	MOTA	1461	C	THR	Α	255	53.477	7 37.035	23.910	1.00 40.09	A
	ATOM	1462	0	THR	A	255	54.430	37.793	23.772	1.00 43.69	A
30	MOTA	1463	N	GLU	А	256	53.617	35.747	24.189	1.00 44.77	A
	MOTA	1464	CA	GLU	Α	256	54.932	35.144	24.382	1.00 49.15	A
	MOTA	1465	CB	GLU	Α	256	54.866	34.143	25.534	1.00 51.24	A
	MOTA	1466	CG	GLU	Α	256	54.514	34.786	26.862	1.00 56.03	Α
•	ATOM	1467	CD	GLU	Α	256	54.053	33.780	27.893	1.00 58.83	A
35	MOTA	1468	OE1	GLU	·A	256	54.766	5 . 32.776	28.107	1.00 62.13	A
	ATOM	1469	OE2	GLU	Α	256	52.979	33.996	28.494	1.00 60.34	A
	MOTA	1470	C	GLU	Α	256	55.475	34.456	23.137	1.00 50.09	A
	MOTA	1471	Ο.	GLU	A	256	56.616	33.995	23.127	1.00 50.42	A
	ATOM	1472	И	LYS	Α	257	54.658	34.389	22.090	1.00 51.21	A
40	ATOM	1473	CA	LYS	Α	257	55.064	33.746	20.845	1.00 51.22	A
	ATOM	1474	CB	LYS	Α	257	56.244	34.502	20.227	1.00 53.28	A
	ATOM	1475	CG	LYS	Α	257	56.558	34.125	18.790	1.00 55.19	A
	ATOM	1476	CD	LYS	Α	257	57.709	34.961	18.253	1.00 57.52	Α
	ATOM	1477	CE	LYS	A	257	57.952	34.694	16.777	1.00 58.52	· А
45	ATOM	1478	NZ	LYS	Α	257	58.290	33.268	16.515	1.00 60.88	A
	ATOM	1479	C.			257	55.467			1.00 50.74	
	ATOM	1480	0			257	56.432		20.577	1.00 52.26	Α
	ATOM	1481	N			258	54.72		22.027	1.00 48.07	
	ATOM	1482	CA			258	54.999		22.402	1.00 46.87	
50	ATOM	1483	СВ			258	55.590		23.812	1.00 48.88	
	ATOM	1484	OG			258	54.743		24.734	1.00 53.14	_
	ATOM	1485	C			258	53.73		22.342	1.00 44.07	
	ATOM	1486	ō			258	52.61		22.417	1.00 44.17	
	ATOM	1487	N			259	53.91		22.204	1.00 38.30	_
55	MOTA	1488	CA			259	52.79		22.127	1.00 34.73	
J J	ATOM	1489	CB			259	52.55		20.684	1.00 34.16	
	ATOM	1490	C			259	53.042		22.977	1.00 32.34	
	MOTA	1491	0			259	54.17		23.086		
	ATOM	1492	И			260	51.97		23.579	1.00 28.58	
	2 2 2 01.7	~					,,				

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	ATOM	1493	CA	CYS	A	260		52	. 056	24.2	44	24.425	1.00	26.27	A
	ATOM	1494	CB	CYS	Α	260		52	.183	24.6	54 ·	25.892	1.00	26.53	A
	ATOM	1495	SG	CYS	A	260		50	.846	25.7	39	26.469	1.00	32.91	A
	ATOM	1496	С	CYS	Α	260		50	. 786	23.4	35	24.224	1.00	22.83	A
5	ATOM	1497	0	CYS	A	260		49	. 892	23.8	56	23.495	1.00	22.14	A
	ATOM	1498	N	LYS	A	261		50	.706	22.2	77	24.868	1.00	20.02	^A
	MOTA	1499	CA	LYS	Α	261		49	.526	21.4	34	24.744	1.00	20.65	A
	MOTA	1500	CB	LYS	A	261	-	49	.619	20.2	43	25.696	1.00	23.28	A
	ATOM	1501	CG	LYS	A	261		50	.716	19.2	53	25.347	1.00	27.44	A
10	ATOM	1502	CD	LYS	A	261		50	.732	18.1	17	26.350	1.00	29.98	A
	MOTA	1503	CE	LYS	Α	261		51	. 922	17.2	03	26.134	1.00	32.34	A
	MOTA	1504	NZ	LYS	Α	261		51	.940	16.1	21	27.153	1.00	33.28	A
	ATOM	1505	C	LYS	A	261		48	.268	22.2	29	25.062	1.00	19.20	A
	ATOM	1506	0	LYS	Α	261		47	. 253	22.0	92	24.387	1.00	18.08	A
15	MOTA	1507	N	SER	A	262		48	.358	23.0	68	26.089	1.00	16.92	A
	MOTA	1508	CA	SER	Α	262		47	.235	23.8	83	26.534	1.00	18.13	A
	ATOM	1509	CB	SER	A	262		47	.644	24.6	98	27.770	1.00	18.27	A
	ATOM	1510	OG	SER	Α	262		46	.517	25.2	58	28.421	1.00	22.53	A
	MOTA	1511	C	SER	Α	262		46	.736	24.8	11	25.424	1.00	16.77	A
20	ATOM	1512	0	SER				45	.591	25.2	54	25.450	1.00	15.69	A
	ATOM	1513	N.	SER				47	. 595	25.1	18	24.456	1.00	16.44	A
	ATOM	1514	CA			263			.175	25.9	70	23.347	1.00	16.89	A
	ATOM	1515	CB			263			.340	26.2		22.382	1.00	18.49	A
	ATOM	1516	OG			263			.402	26.9	09	23.031	1.00	22.10	A
25	ATOM	1517	C			263			.040	25.2		22.612	1.00	17.79	A
	ATOM	1518	ō			263			.099	25.8	98	22.148	1.00	17.57	A
	ATOM	1519	N			264			.119	23.9		22.517	1.00	16.30	A
	ATOM	1520	CA			264			.069	23.1	66	21.836	1.00	16.72	A
	ATOM	1521	CB			264			.483	21.7		21.620	1.00	15.92	A
30	ATOM	1522	CG			264			.544	21.5		20.548	1.00	17.93	Α
50	MOTA	1523		ASP					.642	22.4		19.661	1.00	16.78	A
	ATOM	1524		ASP					.265	20.5		20.579	1.00	16.64	A
	ATOM	1525	C			264			.773	23.1		22.646	1.00	17.67	A
	MOTA	1526	ō			264			.681	23.1		22.076	1.00	18.27	A
35	ATOM	1527	N			265			.898	23.2		23.974	1.00	15.49	A
23	ATOM	1528	CA			265			.730	23.2		24.849	1.00	14.75	A
	ATOM	1529	СВ			265			.147	23.0		26.313	1.00	11.38	A
	ATOM	1530	CG			265			.711	21.6		26.621	1.00	14.04	A
	ATOM	1531		LEU					.249			28.052	1.00	13.96	Α
40	ATOM	1532		LEU					.619	20.6		26.416	1.00	11.62	·A
40	ATOM	1533	. C			265			.999	24.5		24.675	1.00	15.13	Α
	ATOM	1534	ō			265			.777	24.6		24.785	1.00	16.75	Α
	ATOM	1535	N			266			.746	25.6		24.405	1.00	16.08	Α
	MOTA	1536	CA			266			.118	26.9		24.184		16.96	A
45	ATOM	1537	CB			266			.176	28.0		24.023		17.28	A
43		1538	CG			266			.618	29.3		23.521		20.54	A
	ATOM ATOM	1539	CD2			266			.313	30.4		24.301		20.07	A
		1540		TRP					.782	31.4		23.417		20.46	A
	MOTA	1541		TRP					.435	30.8		25.660		20.68	A
50	MOTA	1541		TRP					.270	29.6		22.231		19.53	A
50	MOTA			TRP					.769	30.9		22.163		19.61	A
	ATOM	1543 1544		TRP					.372	32.7		23.850		20.90	A
	ATOM	1544		TRP					.026	32.0		26.091		19.45	A
	MOTA	1545		TRP					.501	33.0		25.031		20.71	A
55	ATOM ATOM	1547	Cnz			266			.284	26.7		22.913		17.22	A
23	ATOM	1548	o			266			.139	27.2		22.863		18.03	A
		1549	N.						. 863	26.3		21.886		17.50	A
	MOTA					267			.155	25.9		20.626		0 16.16	A
	MOTA	1550	CA			267			2.050	25.2		19.621		0 14.28	A
	ATOM	1551	CB	АLA	. A	267		-1 2		40.4	. JU	19.021	T . O.		

	ATOM	1552	C	ALA .	Α	267		39.	901	25.	159	20.8	91	1.0	0.	16.28	A
•	ATOM	1553	0	ALA				38.	835	25.	436	20.3	46	1.0	0	16.46	A
	ATOM	1554	N	LEU .	Α	268			031		144	21.7				16.57	A
	ATOM	1555	CA	LEU					890		299	22.0				17.03	A
. 5	ATOM	1556	CB	LEU					292		260	23.1				15.35	A
,	ATOM	1557	CG	LEU					158		429	23.7				19.00	A
	ATOM	1558		LEU					505		578	22.6				16.17	A
	ATOM	1559		LEU					718		537	24.8				17.49	A
		1560	CDZ	LEU			•		766		179	22.6				15.72	A
10	ATOM			LEU					603		031	22.2				15.72	A
10	ATOM	1561	0														A
	ATOM	1562	N	GLY					119		099	23.5				14.34	A
	ATOM	1563	CA	GLY		, -			124		989	24.0		•		13.39	
	ATOM	1564	С	GLY.					406		808	23.0				14.94	A
	ATOM	1565	0	GLY					193		014	23.1				14.76	A
15	MOTA	1566	N	CYS					146		279	22.0				13.86	A
	ATOM	1567	CA	CYS					539		061	20.9				16.80	A
	ATOM	1568	CB			270 ·			611		634	20.0				15.97	· A
	ATOM	1569	SG	CYS	A	270		38.	751	29.	810	20.7				20.48	A
	ATOM	1570	C	CYS	Α	270		35.	598	27.	175	20.1	40			17.50	A
20	MOTA	1571	0	CYS	A	270		34.	516	27.	604	19.7	41	1.0	0	18.38	A
	ATOM	1572	N	ILE	Α	271		36.	022	25.	939	19.8	87	1.0	0	16.99	A
	MOTA	1573	CA	ILE	Α	271		35.	221	25.	004	19.1	04	1.0	0	16.66	A
	MOTA	1574	CB	ILE	Α	271		36.	038	23.	741	18.7	78	1.0	0	16.53	A
	ATOM	1575	CG2	ILE	Α	271		35.	155	22.	694	18.1	02	1.0	0	16.34	A
25	ATOM	1576	CG1	ILE	Α	271		37.	222	24.	129	17.8	82	1.0	0	15.59	A
	ATOM	1577	CD1	ILE	Α	271		38.	239	23.	018	17.6	90	1.0	0	14.88	A
	ATOM	1578	C	ILE				33.	920.	24.	626	19.8	09	1.0	0	16.74	A
	ATOM	1579	Ō	ILE					865	24.	576	19.1	79	1.0	0	17.12	Α
	ATOM	1580	N	ILE					. 990		357	21.1		1.0	0	16.13	A
30	ATOM	1581	CA	ILE					785	24.	021	21.8	62	1.0	0	18.30	A
50	ATOM	1582	CB	ILE					.097		747	23.3		1.0	0	17.77	A
	ATOM	1583		ILE					796		666	24.1				17.96	A
	ATOM	1584		ILE					877		437	23.4				19.55	A
	ATOM	1585		ILE					446		217	24.8				18.64	Α
35	ATOM	1586	C	ILE					824		207	21.7				19.51	A
55	ATOM	1587	ō	ILE					624		037	21.5				20.44	A
		1588	N	TYR					362		409	21.9				18.52	A
	ATOM	1589	CA	TYR					553		615	21.8				20.48	A
	ATOM			TYR					.418		847	22.1				18.98	A
40	ATOM	1590	CB	TYR					. 663		161	22.1				20.26	. A
40	ATOM	1591	CG	TYR					. 229		709	20.9				20.67	A
	ATOM	1592		TYR					.536		917	20.8				20.98	A
	ATOM	1593		TYR					. 383		857	23.3				19.82	A
	ATOM	1594							. 691		062	23.2				20.62	A
4.5	MOTA	1595		TYR	_							22.0				21.15	A
45	ATOM	1596	CZ	TYR					.271		587					21.86	A
	MOTA	1597	ОН	TYR					.588		776	22.0				21.54	
	MOTA	1598	C	TYR					. 902		730	20.5					. A
	ATOM	1599	0	TYR					.719		049	20.4				22.80	
	ATOM	1600	N	GLN					.676		454 .					21.05	A A
50	ATOM	1601	CA	GLN					.176		538	18.0				21.48	A
	MOTA	1602	CB	GLN					.323		341	17.0				21.41	A
	ATOM	1603	CG	GLN					.934		596	15.6				23.15	A
	MOTA	1604	CD	GLN					.131		588	14.7				24.80	A
	MOTA	1605		GLN					.276		446	15.1				22.51	A
55	ATOM	1606	NE2	GLN					.870		750	13.4				22.96	A
	MOTA	1607	C	GLN					.076		517	17.8		1.0	10	21.51	A
	MOTA	1608	0	GLN	Α	274			.123		806	17.1				20.50	A
	MOTA	1609	N	LEU	A	275		30	.207		324	18.4				21.44	A
	MOTA	1610	CA	LEU	A	275		29	.196	24.	282	18.2	808	1.0	0	20.95	A

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	ATOM	1611	СВ	LEU A	275	29.645	22.958	18.846	1.00 19.11	A ·
	MOTA	1612	CG	LEU A	275	30.775		18.159	1.00 21.43	A
	MOTA	1613		LEU A		31.118		18.963	1.00 17.64	A
	MOTA	1614		LEU A		30.342		16.754	1.00 20.34	A
5	ATOM	1615	С	LEU A		27.860		18.815	1.00 21.32	A
	ATOM	1616	0	LEU A		26.802		18.229	1.00 19.75	A
	ATOM	1617	N	VAL		27.921		19.987	1.00 19.10	A
	ATOM	1618	CA	VAL A		26.724		20.702	1.00 22.47	A
	ATOM	1619	CB	VAL 2		27.011		22.217	1.00 20.87	A
10	ATOM	1620		VAL A		25.742		22.957	1.00 19.68	A
	ATOM	1621		VAL A		27.550		22.766	1.00 19.43	A
	ATOM	1622	C	VAL		26.127		20.211 20.070	1.00 23.89 1.00 24.90	A A
	ATOM	1623	N O	ALA A	276	24.910 26.983		19.965	1.00 24.56	A
15	ATOM ATOM	1624 1625	CA	ALA A		26.533		19.518	1.00 24.72	A
13	ATOM	1626	CB	ALA A		27.504		19.999	1.00 24.72	A
	ATOM	1627	C	ALA A		26.378		18.005	1.00 25.76	A
	ATOM	1628	o	ALA A		25.577		17.502	1.00 26.39	A
	ATOM	1629	N		278	27.142		17.280	1.00 25.13	A
20	ATOM	1630	CA		278	27.062		15.834	1.00 25.58	A
	ATOM	1631	C	GLY Z		28.163	•	15.231	1.00 26.50	A
	ATOM	1632	ō		278	28.374		14.015	1.00 28.17	А
	MOTA	1633	N		279	28.866		16.086	1.00 24.44	A
	ATOM	1634	CA	LEU Z	A 279	29.962	31.130	15.656	1.00 25.21	A
25	ATOM	1635	CB	LEU Z	A 279	29.468	32.575	15.500	1.00 25.78	A
	ATOM	1636	CG	LEU Z	A 279	28.364	32.899	14.490	1.00 28.17	Α
	MOTA	1637	CD1	LEU 2	A 279	27.922	34.344	14.684	1.00 26.60	A
	ATOM	1638		TEA 1		28.862		13.071	1.00 26.52	A
	MOTA	1639	C		A 279	31.093		16.687	1.00 23.47	A
30	ATOM	1640	0		1 279	30.848		17.882	1.00 24.44	Ą
	ATOM	1641	N		1 280	32.349		16.236	1.00 23.35	, A
	MOTA	1642	CD		A 280	32.831		14.855	1.00 22.26 1.00 23.81	A A
	ATOM	1643	CA		A 280	33.464		17.189 16.282	1.00 23.81	A
35	ATOM	1644 1645	CB		A 280 A 280	34.692 34.189		15.073	1.00 24.89	A
33	ATOM ATOM	1646	C		A 280			18.137	1.00 22.69	A
	ATOM	1647	Ö		A 280			17.788	1.00 22.11	A
	ATOM.	1648	N		A 281	•		19.345	1.00 23.06	A
	ATOM	1649	CD		A 281			19.734	1.00 21.37	A
40	ATOM	1650	CA		A 281			20.395	1.00 23.67	A
	ATOM	1651	CB	PRO 2	A 281	34.781	32.751	21.509	1.00 24.89	A
	ATOM	1652	CG	PRO .	A 281	34.749	31.287	21.219	1.00 25.24	A
	ATOM	1653	C	PRO .	A 281	34.481		20.017	1.00 23.75	A
	ATOM	1654	0		A 281			20.317	1.00 21.02	A
45	ATOM	1655	N		A 282			19.379	1.00 22.17	A
	MOTA	1656	CA		A 282			18.998	1.00 23.16	A
	ATOM	1657	CB		A 282			19.406	1.00 21.01	A
	ATOM	1658	CG		A 282			20.822	1.00 22.66	A
	MOTA	1659		PHE .				21.888	1.00 20.06 1.00 20.72	A ·
50	ATOM	1660		PHE .				21.093	1.00 20.72	A A
	MOTA	1661		PHE .				23.206 22.405	1.00 20.97	A
	MOTA	1662			A 282			23.466	1.00 19.58	A
	MOTA MOTA	1663 1664	CZ C		A 282			17.503	1.00 24.39	A
55	ATOM	1665	0		A 282				1.00 25.80	A
55	ATOM	1666	N		A 283			17.142	1.00 24.99	A
	ATOM	1667	CA		A 283			15.741	1.00 26.33	A
	ATOM	1668	CB		A 283			15.316	1.00 28.91	A
	ATOM	1669	CG		A 283			15.724	1.00 30.27	Α

	ATOM	1670	CD	ARG :	A 2	83		31.904	35.493	15.188		33.36	A
	ATOM	1671	NE	ARG .	A 2	283		30.890	36.392	15.733		32.76	A
	ATOM	1672	CZ	ARG .	A 2	283		30.372	36.287	16.952	1.00	34.79	A
	ATOM	1673	NH1	ARG .	A 2	283		30.767	35.317	17.768	1.00	35.77	A
5	ATOM	1674	NH2	ARG .	A 2	283		29.458	37.156	17.359	1.00	36.12	A
	MOTA	1675	C	ARG .	A 2	283		35.328	39.096	15.544	1.00	26.47	A
	ATOM	1676	o ´	ARG .	A 2	283		35.029	39.888	16.438	1.00	26.28	A
	ATOM	1677	N	ALA .	A 2	284		35.818	39.486	14.373	1.00	26.70	A
	ATOM	1678	CA	ALA	A 2	284		36.033	40.899	14.079	1.00	27.84	A
10	ATOM	1679	CB	ALA .	A 2	284		37.188	41.442	14.914	1.00	26.24	A
	MOTA	1680	С	ALA.	A 2	284		36.327	41.077	12.602	1.00	28.35	A
	ATOM	1681	0	ALA	A 2	284		36.560	40.101	11.891	1.00	29.91	A
	ATOM	1682	N	GLY				36.332	42.329	12.153	1.00	29.29	A
	ATOM	1683	CA	GLY	A 2	285		36.577	42.631	10.753	1.00	29.52	A
15	ATOM	1684	C	GLY				37.893	42.156	10.168	1.00	30.12	, A
	ATOM	1685	0	GLY				37.974	41.862	8.976	1.00	30.60	A
	ATOM	1686	N	ASN				38.939	42.097	10.983	1.00	28.49	A
	ATOM	1687	CA	ASN				40.231	41.644	10.489	1.00	26.71	Α
	ATOM	1688	СВ	ASN				41.050	42.825	9.945	1.00	26.11	A
20	ATOM	1689	CG	ASN				41.310	43.900	10.990	1.00	27.83	A
20	MOTA	1690		ASN				41.877	43.631	12.049	1.00	27.84	A
	ATOM	1691		ASN				40.908	45.131	10.685	1.00	25.95	A
	ATOM	1692	C	ASN				40.997	40.924	11.584	1.00	26.03	A
	ATOM	1693	o	ASN				40.540	40.851	12.723	1.00	25.66	A
25	ATOM	1694	N	GLU				42.162	40.391	11.239	1.00	24.81	A
23	ATOM	1695	CA	GLU				42.965	39.662	12.206	1.00	27.59	A
	ATOM	1696	CB	GLU				44.145	38.985	11.510	1.00	30.17	A
	ATOM	1697	CG	GLU				43.776	37.632	10.931	1.00	38.21	A
	ATOM	1698	CD	GLU				44.900	36.998	10.140	1.00	41.86	A
30	ATOM	1699		GLU				46.061	37.036	10.608	1.00	43.08	Α
50	ATOM	1700	OE2					44.612	36.449	9.052	1.00	45.22	A C
	ATOM	1701	C	GLU				43.459	40.485	13.383	1.00	25.05	A
	ATOM	1702	Ō	GLU				43.382	40.030	14.521	1.00	26.41	A
	ATOM	1703	N	TYR	Α	288		43.966	41.685	13.122	1.00	23.04	A
35	ATOM	1704	CA	TYR	Α	288		44.460	42.528	14.205		22.34	A
	MOTA	1705	CB	TYR	Α	288		44.867	43.913	13.691		21.07	A
	MOTA	1706	CG	TYR	Α	288		45.275	44.858	14.805		21.07	A
	MOTA	1707	CD1	TYR	Α	288		46.533	44.762	15.405		21.23	A
	MOTA	1708	CE1	TYR	Α	288		46.891	45.588	16.475		20.43	A
40	MOTA	1709	CD2	TYR	Α	288		44.380	45.809	15.302		22.32	A
	MOTA	1710	CE2	TYR	Α	288		44.725	46.637	16.373		23.28	A
	MOTA	1711	CZ	TYR	A	288		45.981	46.518	16.953		22.96	A
	ATOM	1712	OH	TYR	Α	288		46.316	47.313	18.024		23.18	A
	ATOM	1713	C	TYR	A	288		43.402	42.698	15.288		21.38	A
45	MOTA	1714	0	TYR	Α	288		43.710	42.616	16.473		22.09	A
	MOTA	1715	N	LEU	Α	289		42.159	42.939	14.874		21.88	A
	ATOM	1716	CA	LEU	Α	289		41.055	43.130	15.811		21.98	A
	ATOM	1717	CB	LEU	A	289		39.821	43.673	15.078		22.90	A
	ATOM	1718	CG	LEU	Α	289		39.896	45.130	14.601		26.52	A
50	MOTA	1719	CD1	LEU	Α	289		38.706	45.436	13.696		26.55	A
	ATOM	1720		LEU				39.914	46.071	15.807		23.13	A
	MOTA	1721	C			289		40.686	41.849	16.560		21.24	A
	MOTA	1722	0	LEU	Α	289		40.256		17.715		0 20.72	A
	MOTA	1723	N	ILE	Α	290		40.843		15.900		0 19.62	A
55	ATOM	1724	CA	ILE	Α	290		40.538		16.533		0 18.54	A
	MOTA	1725	СВ	ILE	A	290		40.560		15.509		0 18.52	A
	MOTA	1726	CG:	2 ILE	Α	290		40.503	36.934	16.234		0 17.63	A
	MOTA	1727	CG:	1 ILE	Α	290		39.378		14.545		0 18.88	A
	MOTA	1728	CD:	1 ILE	Α	290	,	39.421	37.483	13.357	1.0	0 19.81	A

	ATOM	1729	C	ILE	Α	290	41.57	8	39.167	17.618	1.00 19.09	A
	MOTA	1730	ō	ILE			41.23		38.788	18.737	1.00 18.20	
	ATOM	1731	N	PHE			42.84		39.376	17.286	1.00 18.76	
				PHE			43.92		39.156	18.247	1.00 20.75	
_	ATOM	1732	CA									
5	ATOM	1733	CB	PHE			45.28		39.434	17.606	1.00 20.71	
	MOTA	1734	CG	PHE			45.64		38.480	16.503	1.00 22.92	
	MOTA	1735	CD1	PHE	Α	291	45.06	5	37.214	16.443	1.00 22.98	A
	ATOM	1736	CD2	PHE	Α	291	46.58	8	38.830	15.543	1.00 22.91	. A
	ATOM	1737	CE1	PHE	A	291	45.42	3	36.310	15.440	1.00 24.51	. A
10	ATOM	1738	CE2	PHE	Α	291	46.95	4	37.931	14.535	1.00 25.54	A
	ATOM	1739	CZ	PHE			46.37		36.670	14.485	1.00 23.29	A
	ATOM	1740	C	PHE			43.73		40:061	19.451	1.00 21.72	
	ATOM	1741	Ö			291	43.99		39.671	20.593	1.00 22.32	
							43.28		41.275	19.178	1.00 23.27	
1.5	ATOM	1742	N	GLN								
15	ATOM	1743	CA	GLN			43.05		42.264	20.216	1.00 24.01	
	MOTA	1744	CB	GLN			42.57		43.559	19.562	1.00 25.77	
	ATOM	1745	CG	GLN	Α	292	42.57	7	44.773	20.447	1.00 28.45	
	MOTA	1746	CD	GLN	Α	292	42.46	9	46.057	19.638	1.00 29.83	A
	MOTA	1747	OE1	GLN	Α	292	41.52	0	46.244	18.872	1.00 27.16	A
20	MOTA	1748	NE2	GLN	Α	292	43.44	9	46.944	19.799	1.00 27.61	. А
	MOTA	1749	С	GLN	Α	292	42.01	.8	41.733	21.204	1.00 22.97	Α
	ATOM	1750	0	GLN			42.20		41.832	22.415	1.00 21.64	A
	ATOM	1751	N	LYS			40.93		41.154	20.687	1.00 21.82	
	ATOM	1752	CA	LYS			39.89		40.612	21.558	1.00 22.18	
25							38.66		40.223	20.740	1.00 22.69	
25	ATOM	1753	CB	LYS							1.00 25.78	
	MOTA	1754	CG			293	37.91		41.407	20.153		
	ATOM	1755	CD	LYS			36.65		40.961	19.429	1.00 27.88	
	ATOM	1756	CE	LYS			35.85		42.161	18.926	1.00 30.85	
	ATOM	1757	NZ	LYS	Α	293	34.61	.2	41.750	18.214	1.00 32.98	B A
30	ATOM	1758	С	LYS	Α	293	40.39	8	39.398	22.343	1.00 21.20) A
	ATOM	1759	0	LYS	Α	293	40.04	1	39.204	23.509	1.00 22.01	. А
	ATOM	1760	N	ILE	Α	294	41.22	26	38.583	21.702	1.00 19.91	. А
	ATOM	1761	CA			294	41.77	74	37.394	22.347	1.00 20.28	a A
	ATOM	1762	CB			294	42.63		36.575	21.349	1.00 18.98	a A
35	ATOM	1763	CG2				43.48		35.550	22.098	1.00 17.70	
<i>JJ</i>	ATOM	1764		ILE			41.71		35.897	20.318	1.00 17.93	
							42.46		35.237	19.178	1.00 16.21	
	ATOM	1765		ILE							1.00 21.94	
	ATOM	1766	C			294	42.61		37.727	23.587		
	MOTA	1767	0			294	42.36		37.199	24.673	1.00 20.86	
40	ATOM	1768	N			295	43.61		38.600	23.439	1.00 21.88	
	ATOM	1769	CA	ILE	Α	295	44.46	51	38.934	24.582	1.00 24.25	
	MOTA	1770	CB	ILE	A	295	45.66	58	39.805	24.175	1.00 23.93	A A
	ATOM	1771	CG2	ILE	Α	295	46.51	L 4	39.066	23.140	1.00 24.63	L A
	ATOM	1772	CG1	ILE	Α	295	45.18	39	41.151	23.637	1.00 24.58	3 A.
45	ATOM	1773	CD1	ILE	Α	295	46.31	L7	42.149	23.433	1.00 26.69) A
	ATOM		C			295	43.72		39.636	25.717	1.00 24.80	
	ATOM	1775	0			295	44.21		39.687	26.842	1.00 24.76	
	ATOM	1776	N			296	42.53		40.173	25.425	1.00 25.33	
							41.74		40.853		1.00 26.80	
50	ATOM	1777	CA			296				26.444	1.00 20.00	
50	ATOM	1778	CB			296	41.17		42.170	25.894		
	ATOM	1779	CG			296	42.24		43.141	25.413	1.00 31.79	
	MOTA	1780	CD			296	41.63		44.410	24.826	1.00 35.56	
	MOTA	1781	CE			296	41.00		45.283	25.900	1.00 39.29	
	ATOM	1782	NZ	LYS	Α	296	40.56	54	46.603	25.357	1.00 41.72	
55	MOTA	1783	С	LYS	A	296	40.59	93	39.958	26.893	1.00 25.50	
	ATOM	1784	0	LYS	À	296	39.77	7,0	40.361	27.713	1.00 24.03	
	ATOM	1785	N			297	40.55	50	38.742	26.349	1.00 25.6	
	ATOM	1786	CA			297	39.50		37.777	26.666	1.00 25.10	
	ATOM	1787	CB			297	39.63		37.285	28.111	1.00 24.80	
	ALVI	1,07	CD			~ 5 ,	22.03	_			_	

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	MOTA	1788	ÇG			297		38.766	36.068	28.460	1.00		A
	MOTA	1789	CD1	LEU	Α	297		39.238	34.852	27.646	1.00	26.70	, A
	ATOM	1790	CD2	LEU	Α	297		38.856	35.777	29.951	1.00	24.84	A
	ATOM	1791	С	LEU	Α	297		38.151	38.459	26.467	1.00	25.11	A
5	ATOM	1792	0			297		37.261	38.378	27.309	1.00		A
,			N			298		38.007	39.127	25.331	1.00		A
	ATOM	1793											
	MOTA	1794	CA			298		36.786	39.847	25.023	1.00		A
	ATOM	1795	CB			298		37.143	41.139	24.291	1.00		A
	MOTA	1796	CG	GLU	Α	298		35.991	42.092	24.108	1.00	31.28	A
10	ATOM	1797	CD	GLU	Α	298		36.419	43.362	23.410	1.00	34.40	A
	ATOM	1798	OE1	GLU	Α	298		37.348	44.027	23.918	1.00	35.90	A
	ATOM	1799	OE2	GLU	Α	298		35.832	43.693	22.359	1.00	36.16	Α
	ATOM	1800	C			298		35.766	39.057	24.207	1.00		A
			ō			298		35.832	39.017	22.979	1.00		A
1.5	ATOM	1801											•
15	MOTA	1802	N.			299		34.825	38.427	24.902	1.00		A
	MOTA	1803	CA			299		33.760	37.663	24.265	1.00		A
	MOTA	1804	CB	TYR	Α	299		34.264	36.304	23.755	1.00	20.13	A
	ATOM	1805	CG	TYR	Α	299		34.348	35.233	24.828	1.00	21.17	A
	ATOM	1806	CD1	TYR	Α	299	,	35.336	35.279	25.810	1.00	19.32	Α
20	ATOM	1807	CE1	TYR	А	299		35.389	34.332	26.826	1.00	19.30	A
	ATOM	1808		TYR				33.410	34.201	24.888	1.00	18.96	Α
	ATOM	1809	CE2	TYR				33.456	33.243	25.907	1.00		'A
											1.00		A
	ATOM	1810	CZ			299		34.449	33.321	26.870			
	MOTA	1811	OH			299		34.511	32.401	27.881	1.00		A
25	MOTA .	1812	C.	TYR				32.699	37.437	25.331	1.00		A
	MOTA	1813	0			299		32.942	37.681	26.506	1.00	26.46	A
	MOTA	1814	N	ASP	Α	300		31.522	36.981	24.927	1.00	26.94	Α
	MOTA	1815	CA	ASP	Α	300		30.467	36.710	25.891	1.00	30.60	A
	ATOM	1816	CB	ASP	Α	300		29.665	37.981	26.179	1.00	35.86	Α
30	MOTA	1817	CG	ASP	Α	300		29.228	38.687	24.923	1.00	42.04	A
	ATOM	1818		ASP				28.450	38.088	24.149	1.00		A
	ATOM	1819		ASP				29.666	39.840		1.00		A
	MOTA	1820	C			300		29.564	35.608	25.363	1.00	•	A
	MOTA	1821	0			300		29.590	35.299	24.172	1.00		A
35	MOTA	1822	N			301		28.778	35.011	26.253	1.00		A
	ATOM	1823	CA	PHE	Α	301		27.884	33.924	25.871	1.00	30.48	A
	ATOM	1824	CB	PHE	Α	301		27.818	32.854	26.968	1.00	29.17	A
	ATOM	1825	CG	PHE	Α	301		29.147	32.279	27.356	1.00	29.29	Α
	ATOM	1826	CD1	PHE	Α	301		29.978	32.949	28.245	1.00	27.31	Α
40	ATOM	1827		PHE				29.560	31.050	26.845	1.00		A
••	ATOM	1828		PHE				31.205	32.403	28.625	1.00		A
				PHE				30.781		27.217	1.00		A
	ATOM	1829							30.498.				
	ATOM	1830	CZ			301		31.605	31.175	28.110	1.00		A
	MOTA	1831	C			301		26.459	34.384	25.619	1.00		A
45	MOTA	1832	0	PHE	Α	301		25.946		26.317	1.00		A
	MOTA	1833	N	PRO	A	302		25.798	33.804	24.607	1.00	33.29	A
	MOTA	1834	CD	PRO	Α	302		26.313	32.943	23.529	1.00	34.04	A
	MOTA	1835	CA	PRO	Α	302		24.415	34.199	24.341	1.00	35.24	A
	ATOM	1836	СВ			302		24.144	33.608	22.959	1.00		Α
50	ATOM	1837	CG			302		25.041	32.413		1.00		A
50													A
	ATOM	1838	C			302		23.567	33.561	25.444	1.00		
	ATOM	1839	0			302		23.935	32.518	25.986	1.00		A
	ATOM	1840	N			303		22.447	34.188	25.783	1.00		A
	ATOM	1841	CA			303		21.572	33.692	26.843	1.00	40.65	A
55	MOTA	1842	CB	ALA	Α	303		20.280	34.506	26.862	1.00	41.66	A
	ATOM	1843	C	ALA	Α	303		21.238	32.197	26.814	1.00	41.25	A
	ATOM	1844	0			303		21.253	31.537	27.854	1.00		A
	ATOM	1845	N			304		20.945	31.665	25.631	1.00		A
			CA			304		20.569	30.258		1.00		A
	MOTA	1846	CA	TH	~	204		20.503	30.430	25.480	1.00	10.00	

	ATOM	1847	CB	ALA	A	304		20.121	30.004	24.040	1.00 41.36	A
	ATOM	1848	C	ALA	Α	304		21.628	29.223	25.876	1.00 39.61	A
	MOTA	1849	0	ALA	Α	304		21.298	28.156	26.395	1.00 40.61	A
	ATOM	1850	N	PHE	A	305		22.891	29.543	25.617	1.00 36.21	Α
5	MOTA	1851	CA	PHE	Α	305		24.022	28.662	25.909	1.00 32.08	A
	MOTA	1852	CB	PHE	A	305		25.259	29.519	26.187	1.00 29.46	A
	MOTA	1853	CG	PHE	A	305		26.536	28.917	25.690	1.00 28.15	A
	MOTA	1854	CD1	PHE	Α	305		27.146	27.875	26.377	1.00 26.20	A
	MOTA	1855	CD2	PHE	A	305		27.127	29.386	24.521	1.00 27.05	A
10	MOTA	1856	CE1	PHE	A	305		28.330	27.308	25.908	1.00 26.92	A
	MOTA	1857	CE2	PHE	Α	305		28.312	28.826	24.042	1.00 26.62	A
	MOTA	1858	CZ	PHE	Α	305		28.914	27.786	24.737	1.00 26.61	A
	MOTA	1859	C	PHE	A	305		23.811	27.664	27.057	1.00 30.09	A
	MOTA	1860	0	PHE	A	305		23.518	28.051	28.187	1.00 31.51	A
15	MOTA	1861	N	PHE	A	306		23.964	26.378	26.758	1.00 27.01	A
	MOTA	1862	CA	PHE	Α	306		23.801	25.334	27.769	1.00 26.30	A
	ATOM	1863	CB	PHE	Α	306		24.157	23.970	27.170	1.00 25.03	A
	MOTA	1864	CG	PHE	Α	306		23.548	23.725	25.815	1.00 27.24	Α
	ATOM	1865	CD1	PHE	Α	306		22.170	23.831	25.622	1.00 28.40	A
20	ATOM	1866	CD2	PHE	Α	306		24.350	23.386	24.728	1.00 27.84	Α
	MOTA	1867	CE1	PHE	A	306		21.601	23.603	24.365	1.00 28.05	A
	MOTA	1868	CE2	$_{ m PHE}$				23.792	23.155	23.465	1.00 28.31	A
	ATOM	1869	CZ	PHE	A	306		22.415	23.263	23.283	1.00 28.00	Α
	ATOM	1870	С	PHE	Α	306		24.711	25.652	28.961	1.00 26.23	A
25	ATOM	1871	0	PHE	Α	306		25.927	25.775	28.811	1.00 25.59	A
	ATOM	1872	N	PRO				24.125	25.796	30.163	1.00 26.67	A
	MOTA	1873	· CD	PRO	A	307		22.685	25.625	30.430	1.00 27.95	A
	MOTA	1874	CA	PRO	Α	307		24.842	26.110	31.405	1.00 26.59	Α.
	ATOM	1875	CB	PRO	A	307		23.795	25.832	32.481	1.00 26.14	A
30	MOTA	1876	CG	PRO	A	307		22.531	26.250	31.803	1.00 27.86	A
	MOTA	1877	С	PRO	A	307		26.145	25.355	31.659	1.00 25.58	A
	ATOM	1878	0	PRO				27.189	25.964	31.900	1.00 22.65	A
	MOTA	1879	N	LYS				26.085	24.031	31.620	1.00 24.46	A
	MOTA	1880	CA	LYS				27.274	23.232	31.867	1.00 23.91	A
35	MOTA	1881	CB	LYS				26.887	21.760	32.024	1.00 23.25	A
	MOTA	1882	CG	LYS				26.062	21.532	33.285	1.00 28.49	A
	MOTA	1883	CD	LYS				25.618	20.093	33.466	1.00 30.17	A
	MOTA	1884	CE	LYS				24.760	19.973	34.722	1.00 33.12	A
	MOTA	1885	NZ	LYS				24.122	18.636	34.860	1.00 34.13	A A
40	MOTA	1886	C	LYS				28.314	23.426	30.769	1.00 22.84	
	MOTA	1887	0	LYS				29.514	23.411	31.042	1.00 22.46	A A
	MOTA	1888	N	ALA				27.861	23.621	29.534	1.00 21.59	A A
•	MOTA	1889	CA			309	•	28.792	23.848	28.432	1.00 20.02	A
	MOTA	1890	CB			309		28.056	23.856	27.106	1.00 18.80 1.00 21.41	A
45	ATOM	1891	C	ALA				29.481	25.191	28.662		A
	MOTA	1892	0	ALA				30.680	25.335	28.427	1.00 21.39	A
	MOTA	1893	N ·			310		28.717	26.179	29.121	1.00 21.39	A
	MOTA	1894	CA			310		29.290	27.494	29.388	1.00 22.02	A
	ATOM	1895	CB			310		28.213	28.479	29.854	1.00 22.39 1.00 25.30	Ā
50	ATOM	1896	CG			310		28.806	29.756	30.436	1.00 28.33	A
	ATOM	1897	CD			310		27.780	30.852	30.664	1.00 28.33	A
	ATOM	1898	NE			310		28.420	32.039	31.230	1.00 30.10	A
	ATOM	1899	CZ			310		27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900		ARG				26.719	33.477	30.634 31.742	1.00 31.19	A
55	MOTA	1901		ARG		310		28.567	34.277 27.388	31.742	1.00 30.45	A.
	MOTA	1902	C					30.376			1.00 21.03	A
	MOTA	1903	O N			310		31.464	27.949 26.677	30.311 31.541	1.00 20.50	A
	ATOM	1904	N CA	•		311 311		30.074	26.577	32.615	1.00 20.18	A
	MOTA	1905	ŲН	ADE	м			31.043	20.312	32.013	1.00 20.20	

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	ATOM	1906	CB	ASP			30.460	25.649	33.739	1.00 20.39	A
	MOTA	1907	CG	ASP			31.439	25.446	34.881	1.00 23.35	A
	MOTA	1908		ASP			32.158	24.428	34.885	1.00 24.91	A
_	ATOM	1909		ASP			31.500	26.312	35.776	1.00 26.96	A
5	ATOM	1910	C	ASP			32.322	25.877	32.073	1.00 19.73	A
	ATOM	1911	0	ASP			33.422	26.289	32.439	1.00 19.30	. A
	ATOM	1912	N CA	LEU			32.179	24.891	31.188	1.00 16.32 1.00 16.66	A
	ATOM	1913 1914	CB	LEU			33.349	24.226 23.035	30.611 29.744	1.00 16.88	A A
10	ATOM ATOM	1914	CG	LEU			32.927 34.050	22.320	28.974	1.00 10.12	A
10	ATOM	1916		LEU			35.192	21.935	29.912	1.00 14.75	A
	ATOM	1917		LEU			33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	C	LEU			34.181	25.189	29.774	1.00 16.61	A
	ATOM	1919	ō	LEU			35.402		29.910	1.00 16.20	A
15	ATOM	1920	N	VAL			33.515	25.949	28.908	1.00 16.20	A
	ATOM	1921	CA	VAL	A	313	34.207	26.907	28.058	1.00 15.37	Α
	ATOM	1922	CB	VAL	A	313	33.216	27.648	27.130	1.00 16.42	A
	MOTA	1923	CG1	VAL	A	313	33.915	28.796	26.426	1.00 16.93	A
	MOTA	1924	CG2	VAL	Α	313	32.644	26.672	26.103	1.00 17.88	A
20	MOTA	1925	С	VAL	A	313	34.960	27.923	28.911	1.00 17.39	. A
	MOTA	1926	0	VAL	A	313	36.093	28.294	28.591	1.00 18.00	A
	ATOM	1927	N	GLU			34.342	28.364	30.004	1.00 17.61	A
	MOTA	1928	CA	GLU			34.986	29.331	.30.885	1.00 20.43	A
	MOTA	1929	CB	GĻŪ			34.009	29.816	31.959	1.00 22.14	A
25	ATOM	1930	CG	GLU			32.800	30.550	31.396	1.00 26.52	A
	ATOM	1931	CD	GLU			31.852	31.025	32.478	1.00 31.26 1.00 33.48	A A
	MOTA	1932		GLU			31.580	30.246	33.417 32.387	1.00 33.48	A
	MOTA	1933 1934	C C	GLU			31.370 36.217	32.173 28.721	31.539	1.00 19.15	A
30	ATOM ATOM	1935	0	GLU			37.134	29.433	31.934	1.00 21.47	A
50	ATOM	1936	N	LYS			36.245	27.400	31.651	1.00 19.51	A
	ATOM	1937	CA	LYS			37.394	26.749	32.258	1.00 19.17	A
	ATOM	1938	СВ	LYS			36.946	25.514	33.043	1.00 18.84	A
	ATOM	1939	CG	LYS			36.280	25.885	34.368	1.00 19.62	. A
35	MOTA	1940	CD	LYS	Α	315	35.653	24.696	35.073	1.00 19.22	A
	MOTA	1941	CE	LYS	Α	315	35.070	25.095	36.427	1.00 21.00	Α
	MOTA	1942	NZ	LYS	A	315	36.119	25.552	37.381	1.00 19.53	. A
	ATOM	1943	С	LYS	A	315	38.452	26.393	31.218	1.00 18.96	A
	MOTA	1944	0	LYS	Α	315		25.873	31.561	1.00 19.85	A
40	MOTA	1945	N			316	38.164	26.691	29.950	1.00 17.08	A
	ATOM	1946	CA			316	39.102	26.429	28.854	1.00 16.41	A
	MOTA	1947	CB			316	38.414	25.636	27.738	1.00 13.81	A
	ATOM	1948	CG			316	38.028	24.201	28.115	1.00 14.39	A A
4.5	ATOM	1949		LEU			37.139	23.597	27.031	1.00 12.38	A
45	MOTA	1950		LEU			39.302 39.652	23.373 27.743	28.309 28.290	1.00 12.77 1.00 17.12	A
	ATOM	1951 1952	С О			316 316	40.851	27.860	28.023	1.00 17.12	A
	MOTA MOTA	1952	N			317	38.780	28.729	28.105	1.00 16.27	A
	ATOM	1954	CA			317	39.228	30.022	27.596	1.00 17.52	· A
50	ATOM	1955	CB			317	38.083	30.752	26.887	1.00 16.37	A
50	ATOM	1956	CG			317	37.448	29.973	25.727	1.00 18.81	A
	ATOM	1957		LEU			36.415	30.851	25.018	1.00 16.47	A
	ATOM	1958		LEU			38.528	29.526	24.741	1.00 17.87	Α
	ATOM	1959	С			317	39.745	30.841	28.774	1.00 18.27	Α
55	MOTA	1960	0	LEU	A	317	39.078	31.753	29.273	1.00 18.58	Α
	MOTA	1961	N	VAL	A	318	40.937	30.475	29.229	1.00 18.02	A
	MOTA	1962	CA			318	41.593	31.141	30.342	1.00 18.85	A
	MOTA	1963	CB			318	41.846	30.153	31.500	1.00 19.91	A
	ATOM	1964	CG1	VAL	Α	318	42.590	30.848	32.634	1.00 20.01	_ A

	MOTA	1965	CG2	VAL	Α	318		40	.520	29.	584	31.990	1.0	0 19	44	A
	MOTA	1966	С	VAL	Α	318		42	. 923	31.	657	29.811	1.0	0 19	67	A
	MOTA	1967	0	VAL	Α	318		43	.690	30.	902	29.208	1.0	0 18	26	A
	MOTA	1968	N	LEU	Α	319		43	.197	32.	939	30.028	1.0	0 20	07	A
5	MOTA	1969	CA	LEU	Α	319		44	.436	33.	533	29.538	1.0	0 20	98	A
	MOTA	1970	CB	LEU	Α	319		44	.521	35.	002	29.968	1.0	0 21	64	A
	ATOM	1971	CG	LEU	Α	319		43	.418	35.	908	29.408	1.0	0 24	.38	A
	MOTA	1972	CD1	LEU	Α	319		43	.606	37.	332	29.935	1.0	0 23	28	A
	ATOM	1973	CD2	LEU	Α	319		43	.453	35.	887	27.875	1.0	0 24	.33	A
10	ATOM	1974	С	LEU				45	.680	32.	774	29.994	1.0	0 20	.38	A
	ATOM	1975	0	LEU					.568	32.		29.192	1.0	0 21	.34	A
	ATOM	1976	N	ASP					.742	32.		31.280	1.0	0 20	. 22	A
	ATOM	1977	CA	ASP			•	-	.879	31.		31.833		0 20		A
	ATOM	1978	СВ	ASP					.842	31.		33.365	1.0	0 20	76	Α
15	ATOM	1979	CG	ASP					.049	31.		34.004		0 21		A
	ATOM	1980		ASP					.669	30.		33.367		0 23		A
	ATOM	1981		ASP					.371	31.		35.159		0 23		A
	ATOM	1982	C	ASP					.814	30.		31.367		0 20		. A
	ATOM	1983	o	ASP					.988	29.		31.840		0 20		A
20	ATOM	1984	N	ALA					.700	29.		30.451		0 20		A
20	MOTA	1985	CA	ALA					.733	28.		29.903		0 22		A
	ATOM	1986	CB	ALA					.860	28.		28.881		0 20		A
	ATOM	1987	C	ALA					.858	27.		30.940		0 21		· A
			o	ALA					.482	26.		30.665		0 21		A
25	MOTA	1988 1989	N	THR					.372	27.		32.127		0 20		A
23	ATOM	1999		THR					.531			33.167		0 20		A
	ATOM		CA CB						.670		051	34.146		0 19		A
	ATOM	1991		THR			-		.341	28.		34.848		0 20		A
	MOTA	1992		THR							233 249	33.394		0 21		A
20	ATOM	1993	CG2	THR					.981 .264	26.		33.983		0 19		A
30	MOTA	1994	C	THR						25.		34.894		0 21		A
	ATOM	1995	0	THR					.235			33.661		0 19		A
	ATOM	1996	N	LYS					.216	27.	122	34.392		0 21		A
	ATOM	1997	CA	LYS					.962			35.030		0 23		A
25	MOTA	1998	CB	LYS					.580		460	36.084		0 28		A
35	MOTA	1999	CG	LYS					.562		933			0 33		A
	ATOM	2000	CD	LYS					.055		177	36.799				A
	MOTA	2001	CE	LYS					.087		678	37.802		0 36		A
	ATOM	2002	NZ	LYS					.532		569	38.693		00 37 00 20		Ą
40	ATOM	2003	C	LYS			•		.806		614	33.539				Ã
40	MOTA	2004	0	LYS					.649		757	33.915 32.392		0 20		A
	ATOM	2005	N .	ARG					.114		019	31.531		00 19 00 17		A
	MOTA	2006	CA	ARG					.060		494					A
	ATOM	2007	CB	ARG					.461		609	30.061 29.603		00 15 00 17		A
4.5	ATOM	2008	CG	ARG					.534		050	28.172		0 19		Ā
45	MOTA	2009	CD	'ARG					.996		194	27.944		0 16		A
	ATOM	2010	NE	ARG					.438	28.						
	ATOM	2011	CZ	ARG					.410		908	27.108		0 19		A A
	ATOM	2012		ARG					.045		978	26.398		0 14		A
	MOTA	2013		ARG					.774	30.		27.015		0 16		A
50	ATOM	2014	С	ARG					.762		046	31.883		0 18		A
	MOTA	2015	0	ARG					.673		222	32.006		0 18		A A
	ATOM	2016	N	LEU					.479		748	32.055		0 18		A
•	ATOM	2017	CA	LEU					.050		403	32.395		0 17		A
<i></i>	ATOM	2018	CB	LEU					.523		335	32.425		0 17		A
55	MOTA	2019	CG	LEU					.896		125	33.116		0 15		A
	ATOM	2020		LEU					.392		048	34.557		00 15 00 16		A
	MOTA	2021		LEU							255	33.084				· A
	ATOM	2022	C	LEU					.599		433	31.356		0 18		A
	MOTA	2023	0	LEU	A	325		4 J	.347	۷1.	586	30.157	Τ.(0 18	. 48	A

	ATOM	2024	N	GLY A	326		42.354	20.439	31.821	1.00 18.18	A
	ATOM	2025	CA	GLY A	326		42.931	19.462	30.915	1.00 16.36	A
	ATOM	2026	C	GLY A	326		44.443	19.558	30.807	1.00 19.15	Α
	ATOM	2027	0	GLY A	326		45.093	18.592	30.404	1.00 19.52	Α
5	ATOM	2028	N	CYS A	327		45.016	20.708	31.161	1.00 18.16	A
	ATOM	2029	CA	CYS A	327		46.463	20.867	31.075	1.00 19.30	A
	MOTA	2030	ĊВ	CYS A	327		46.856	22.350	31.058	1.00 20.22	A
	MOTA	2031	SG	CYS A	327		46.782	23.200	32.649	1.00 21.97	Α
	MOTA	2032	С	CYS A	327		47.169	20.157	32.228	1.00 20.22	Α
10	MOTA	2033	0	CYS A	327		46.561	19.828	33.246	1.00 17.92	A
	ATOM	2034	И	GLU A	328		48.463	19.933	32.053	1.00 20.51	A
	ATOM	2035	CA	GLU A	328		49.274	19.244	33.042		A
	ATOM	2036	CB	GLU A			50.710	19.139	32.507	1.00 28.68	A
	ATOM	2037	CG	GLU A	328		50.754	18.367	31.175	1.00 38.24	A
15	MOTA	2038	$^{\rm CD}$	GLU A	328		52.067	18.500	30.414	1.00 43.23	A
	MOTA	2039		GLU A			52.535		30.218	1.00 46.22	A
	MOTA	2040	OE2				52.618	17.459	29.991	1.00 44.90	A
	MOTA	2041	C	GLU A			49.234	19.876	34.435	1.00 22.11	A
•	MOTA	2042	· O	GLU A			49.147	19.161	35.437	1.00 20.27.	A
20	MOTA	2043	N	GLU A	•		49.276	21.204	34.506	1.00 18.40	A
	ATOM	2044	CA	GLU A			49.248	21.875	35.801	1.00 20.13	A
	MOTA	2045	CB	GLU A			49.587	23.363	35.657	1.00 20.36	A
	MOTA	2046	CG	GLU A			51.014	23.651	35.190	1.00 24.05	A
	ATOM	2047	CD	GLU A			51.191	23.518	33.688	1.00 25.93	A.
25	MOTA	2048		GLU A			50.213	23.154	32.995	1.00 26.61	A A
	ATOM	2049		GLU A			52.311	23.781	33.198	1.00 27.19	A
	ATOM	2050	C	GLU A			47.890	21.718	36.480	1.00 19.36 1.00 18.74	A
	MOTA	2051	0	GLU A			47.775	21.879	37.694	1.00 18.74	. A
••	MOTA	2052	И	MET A			46.863	21.415	35.691 36.229	1.00 17.28	. A
30	MOTA	2053	CA	MET A			45.520	21.220	35.294	1.00 10.30	A
	MOTA	2054	CB	MET A			44.474	21.833	35.234	1.00 17.05	A
	ATOM	2055	CG	MET A			44.460	23.365 24.026	36.979	1.00 26.78	A
	ATOM	2056	SD	MET A		•	44.186 42.435	23.712	37.186	1.00 24.69	A
25	MOTA	2057	CE	MET A			45.257	19.730	36.422	1.00 14.30	A
35	ATOM	2058	C	MET A			44.127	19.304	36.629	1.00 15.39	A
	MOTA	2059	0	GLU A			46.327	18.949	36.346	1.00 15.60	A
	MOTA	2060	N	GLU A			46.289	17.501	36.531	1.00 17.08	A
	MOTA	2061	CA CB	GLU A			45.607	17.155	37.862	1.00 17.00	A
40	ATOM	2062 2063	CB	GLU A			46.070	18.027	39.038	1.00 17.46	А
40	ATOM ATOM	2063	CD	GLU A			47.591	18.179	39.145	1.00 20.16	A
	ATOM	2065		GLU A			48.034	19.073	39.896	1.00 21.39	A
	ATOM	2066		GLU A			48.345	17.420	38.500	1.00 18.87	A
	ATOM	2067	C	GLU A			45.697	16.658	35.398	1.00 17.80	A
45	ATOM	2068	ō	GLU A			45.107	15.602	35.636	1.00 20.40	A
-13	ATOM	2069	N	GLY A			45.844	17.133	34.167	1.00 16.23	A
	MOTA	2070	CA	GLY A			45.420	16.353	33.015	1.00 14.10	A
	ATOM	2071	C	GLY A			43.982	16.154	32.596	1.00 13.54	A
	ATOM	2072	Ö	GLY A			43.063	16.864	33.017	1.00 11.96	A
50	ATOM	2073	Ŋ	TYR A			43.804	15.141	31.750	1.00 14.37	A
50	ATOM	2074	CA	TYR A			42.510	14.806	31.182	1.00 13.56	Α
	ATOM	2075	СВ	TYR A			42.722	13.892	29.968	1.00 15.00	A
	ATOM	2076	CG	TYR ·			43.153	14.683	28.752	1.00 16.46	A
	ATOM	2077		TYR F			42.206	15.172	27.849	1.00 15.29	A
55	MOTA	2078		TYR F			42.573	16.002	26.794	1.00 13.42	A
	MOTA	2079		TYR F			44.490	15.039	28.561	1.00 14.91	A
	MOTA	2080	CE2	TYR F	333	-	44.872	15.877	27.499	1.00 14.87	A
	MOTA	2081	CZ	TYR A	333		43.902	16.353	26.626	1.00 15.61	A
	ATOM	2082	OH	TYR A	333		44.244	17.197	25.599	1.00 17.29	A

	ATOM	2083	С	TYR .	A	333	41.47	0	14.230	32.127	1.00	15.23	A
	ATOM	2084	0	TYR .	A	333	40.27	8	14.323	31.846	1.00	16.63	A
•	ATOM	2085	N	GLY .	A.	334	41.90		13.650	33.244		15.50	A
	ATOM	2086	CA	GLY :	A	334	40.95		13.100	34.202		15.07	A
5	ATOM	2087	C			334 /	39.92		14.146	34.616		16.40	. A
-	ATOM	2088	0	GLY			38.72		13.946	34.433		15.05	A
	ATOM	2089	N	PRO .			40.36		15.278	35.184		14.96	A
	ATOM	2090	CD	PRO			41.72		15.531	35.689		15.88	A
	ATOM	2091	CA	PRO .			39.44		16.339	35.606		15.29	A
10	ATOM	2092	CB	PRO .			40.38		17.397	36.178		13.19	A
10	ATOM	2093	CG	PRO			41.48		16.569	36.758		13.81	A
	ATOM	2094	C	PRO :			38.59		16.877	34.448		15.84	A
	ATOM	2095	Ö	PRO			37.42		17.204	34.631		14.84	A
	ATOM	2096	И	LEU .			39.18		16.971	33.257		16.12	A
15		2096	CA	LEU .			38.45		17.465	32.094		15.52	A
13	ATOM	2097		LEU .					17.653	30.898		14.39	A
	ATOM		CB				39.39						A
		2099	CG	LEU .			38.77		17.991	29.538		15.46	A
	ATOM	2100		LEU :			37.83		19.182	29.662		11.25	A
20	ATOM	2101		LEU .			39.88		18.285	28.528		14.11	A
20	ATOM	2102	C.	LEU .			37.32		16.508	31.714		16.28	A
	ATOM	2103	0	LEU .			36.17		16.921	31.540		15.51	A
	MOTA	2104	N	LYS .			37.64		15.225	31.592		17.22	A
	ATOM	2105	CA	LYS .			36.62		14.243	31.235		17.39 17.68	A
25	MOTA	2106	CB	LYS .			37.29		12.900	30.921 29.676		22.31	A
25	ATOM	2107	CG	LYS .			38.17		12.994			24.60	
	ATOM	2108	CD	LYS .			39.21		11.892	29.592 29.189		24.76	A
	ATOM	2109	CE	LYS .			38.62		9.560	28.997		25.05	A
	ATOM	2110 2111	NZ	LYS .			39.71			32.342		17.33	A
20	ATOM		C				35.57		14.096	32.090		14.42	A
30	ATOM	2112	0	LYS .			34.45		13.652 14.500	33.559		15.83	A
	ATOM	2113	N	ALA			35.92			34.674		17.52	A
	ATOM	2114	CA	ALA .			34.98		14.395 14.167	35.980		19.68	A
	MOTA	2115	CB	ALA .			35.74 34.09		15.621	34.804		18.83	A
25	ATOM	2116	С 0	ALA .			33.25		15.687	35.695		18.94	A
35	MOTA	2117	N	HIS .			34.26		16.596	33.918		19.42	A
	MOTA	2118 2119	CA	HIS .			33.43		17.796	34.004		19.28	A
	ATOM ATOM	2119	CB			339	33.86		18.819	32.949		19.20	A
	ATOM	2121	CG	HIS .			33.16		20.134	33.074		20.26	A
40		2121		HIS .			33.54		21.299	33.649		18.95	A
40	ATOM	2123		HIS .			31.88		20.340	32.612		19.10	A
	ATOM ATOM	2123		HIS .			31.50		21.576	32.896		22.19	A
	ATOM	2124		HIS .			32.50		22.179	33.525		21.98	A
	ATOM	2125	C	HIS .			31.95		17.448	33.845		19.13	A
45										33.061			
45	ATOM	2127	0				31.59		18.125	34.606		19.80	A
	ATOM	2128 2129	N CD	PRO .			31.07 31.42		19.119	35.640		19.08	A
	ATOM ATOM	2129	CA	PRO .			29.63		17.900	34.569		20.52	A
		2130		PRO .			29.09		19.058	35.396		20.74	A
50	ATOM ATOM	2132	CB CG			340	30.14		19.207	36.454		19.20	A
50	ATOM	2132	C	PRO			29.00		17.834	33.176		21.42	A
	ATOM	2134	0	PRO			28.04		17.088	32.955		22.48	A
				PHE			29.52		18.606	32.237		21.33	A
	ATOM ATOM	2135 2136	N CA	PHE			28.98	- 1	18.610	30.886		21.57	A
55	ATOM	2136	CB	PHE			29.73		19.624	30.017		21.64	A
رر	ATOM	2137	CG	PHE			29.20		19.740	28.613		23.18	A
	MOTA	2136		PHE			27.90		20.171	28.382		22.58	A
	ATOM	2139		PHE			30.01		19.431	27.522		21.95	A
	ATOM	2140		PHE			27.41		20.292	27.082		23.54	A
		~ ~ 4 4											

	ATOM	2142	CE2	PHE	A 341		29.533	19.548	26.220	1.00 21.83	Α
	ATOM	2143	CZ	PHE	A 341		28.228	19.980	25.998	1.00 23.23	A
	ATOM	2144	C	PHE	A 341	•	29.055	17.226	30.237	1.00 21.84	A
	ATOM	2145	0	PHE	A 341		28.232	16.896	29.389	1.00 20.37	A
5	ATOM	2146	N	PHE	A 342		30.034	16.422	30.640	1.00 20.51	Α
_	ATOM	2147	CA	PHE	A 342		30.221	15.085	30.077	1.00 23.01	A
	ATOM	2148	CB		A 342		31.710	14.809	29.850	1.00 18.00	A
	MOTA	2149	CG		A 342		32.398	15.812	28.971	1.00 17.05	A
	ATOM	2150			A 342		32.010	15.987	27.652	1.00 17.78	A
10	ATOM	2151			A 342		33.487	16.534	29.450	1.00 15.72	A
10	MOTA	2152			A 342		32.702	16.867	26.811	1.00 18.08	Α
	ATOM	2152			A 342		34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ		A 342		33.790	17.578	27.298	1.00 16.56	Α
		2155	C		A 342		29.679	13.972	30.976	1.00 24.95	A
16	MOTA		0		A 342		30.002	12.798	30.777	1.00 23.95	A
15	ATOM	2156	N		A 343		28.861	14.333	31.958	1.00 27.35	A
	ATOM	2157	CA		A 343		28.325	13.349	32.897	1.00 30.28	Α
	MOTA	2158			A 343		27.187	13.964	33.716	1.00 32.20	A
	ATOM	2159	CB		A 343		26.581	12.991	34.714	1.00 39.71	A
-00	ATOM	2160	CG				25.628	13.661	35.688	1.00 44.72	A
20	ATOM	2161	CD		A 343		24.661	14.314	35.234	1.00 47.55	A
	MOTA	2162			A 343			13.526	36.911	1.00 46.89	A
	ATOM .	2163			A 343		25.847 27.852	12.017	32.305	1.00 28.98	A
	ATOM	2164	C		A 343		28.225	10.952	32.800	1.00 31.73	A
0.5	ATOM	2165	0		A 343		27.037	12.067	31.258	1.00 26.09	A
25	ATOM	2166	N	_	A 344		26.520	10.838	30.656	1.00 28.36	A
	MOTA	2167	CA CB		A 344		25.129	11.089	30.067	1.00 28.73	A
	MOTA	2168	OG		A 344		25.203	11.942	28.940	1.00 30.91	Α
	ATOM	2169	C		A 344		27.407	10.214	29.577	1.00 27.66	A
20	ATOM	2170	0		A 344		26.987	9.281	28.900	1.00 28.66	A
30	ATOM	2171	N		A 345		28.627	10.715	29.419	1.00 26.75	A
	ATOM	2172 2173	CA		A 345		29.534	10.183	28.402	1.00 23.44	A
	ATOM		CB		A 345		30.565	11.256	27.950	1.00 23.10	Α
	ATOM	2174 2175			A 345		31.589	10.631	26.995	1.00 22.24	A
35	ATOM	2176	CG2		A 345		29.854	12.418	27.275	1.00 20.05	Α
33	MOTA ATOM	2177	C		A 345		30.326	8.957	28.855	1.00 24.26	A
	ATOM	2178	o		A 345		30.876	8.930	29.960	1.00 22.83	A
	ATOM	2179	N		A 346		30.374	7.942	27.997	1.00 21.77	A
	ATOM	2180	CA		A 346		31.153	6.740	28.272	1.00 23.70	A
40	ATOM	2181	CB		A 346		30.391	5.455	27.857	1.00 26.53	\mathbf{A}_{\cdot}
40	ATOM	2182			A 34		29.248		28.706	1.00 29.98	A
	MOTA	2183	CG2		A 34		31.289	4.231	27.990	1.00 24.28	A
	MOTA	2184	C		A 34		32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	Ö		A 34		32.306	6.827	26.160	1.00 24.50	A
45	ATOM	2186	Ŋ		A 34	_	33.508	7.270	28.013	1.00 22.98	A
73	ATOM	2187	CA		A 34		34.744	7.569	27.300	1.00 23.81	A
	ATOM	2188	CB		A 34		35.683	8.352	28.219	1.00 22.54	A
	ATOM	2189	CG		A 34		35.128	9.658	28.693	1.00 20.61	A
	ATOM	2190			A 34		35.257	10.927	28.040	1.00 19.11	A
50	ATOM	2191			A 34		34.581	11.881	28.838	1.00 18.39	A
50	MOTA	2192			A 34		35.878	11.351	26.858	1.00 18.16	A
	ATOM	2193			A 34		34.397	9.883	29.828	1.00 18.35	A
	ATOM	2194			A 34		34.065	11.218	29.923	1.00 19.51	A
	ATOM	2195			A 34		34.510	13.234	28.491	1.00 16.88	A
55	ATOM	2196			A 34		35.808	12.701	26.511	1.00 17.23	A
55	MOTA	2197	CH		A 34		35.127	13.624	27.327	1.00 18.16	A
	ATOM	2198	C		A 34		35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	0.		A 34		36.304	6.654	25.742	1.00 24.67	A
	ΔTOM	2200			A 34		35.360			1.00 27.10	A

	MOTA	2201	CA	ALA	A	348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	CB	ALA	Α	348	35.899	2.869	27.636	1.00 27.09	A
	ATOM	2203	C	ALA	A	348	35.895	3.620	25.256	1.00 27.18	A
	ATOM	2204	0	ALA	Ą	348	36.830	3.148	24.613	1.00 29.41	A
5	ATOM	2205	N	asn	Α	349	34.682	3.769	24.735	1.00 26.55	A
	MOTA	2206	CA	ASN	A	349	34.418	3.310	23.375	1.00 27.28	A
	MOTA	2207	CB	ASN			33.700	1.962	23.444	1.00 29.37	A
•	MOTA	2208	CG	ASN			32.299	2.088	24.013	1.00 30.92	A
	MOTA	2209		ASN			32.045	2.942	24.859	1.00 30.17	A
10	MOTA	2210		ASN			31.386	1.237	23.553	1.00 33.52	A
	MOTA	2211	С	ASN			33.599	4.265	22.509	1.00 26.47	A
	ATOM	2212	0	ASN			32.669	3.843	21.819	1.00 25.87	. A
	MOTA	2213	N	LEU			33.947	5.543	22.518	1.00 24.45	A.
	ATOM	2214	CA	LEU			33.203	6.510	21.721	1.00 23.14	· A
15	ATOM	2215	CB	LEU			33.837	7.898	21.848	1.00 23.22 1.00 21.05	A A
	ATOM	2216	CG	LEU			33.659	8.605	23.191 23.293	1.00 21.05	A
	ATOM	2217		LEU			34.646	9.756	23.293	1.00 19.38	· A
	ATOM	2218		LEU			32.220	9.094	20.240	1.00 22.60	A
20	ATOM	2219	C	LEU			33.082	6.152 6.296	19.650	1.00 21.15	A
20	ATOM	2220	Й	HIS			32.011 34.165	5.689	19.627	1.00 23.13	A
	MOTA	2221 2222	CA	HIS			34.105	5.387	18.204	1.00 27.83	A
	MOTA MOTA	2222	CB	HIS			35.506	5.325	17.596	1.00 29.36	A
	ATOM	2223	CG	HIS			36.082	3.950	17.493	1.00 32.07	A
25	ATOM	2225		HIS			36.611	3.128	18.431	1.00 32.39	A
23	ATOM	2226		HIS			36.197	3.285	16.291	1.00 33.02	A
	MOTA	2227		HIS			36.775	2.113	16.493	1.00 33.58	· A
	ATOM	2228		HIS		•	37.036	1.992	17.782	1.00 31.76	A
	ATOM	2229	C			351	33.258	4.144	17.874	1.00 28.12	A
30 -	ATOM	2230	0			351	33.015	3.847	16.707	1.00 29.49	A
	ATOM	2231	N			352		3.442	18.908	1.00 29.28	Α
	ATOM	2232	CA	GLN	Α	352	31.963	2.255	18.726	1.00 29.67	Α
•	MOTA	2233	CB	GLN	A	352	32.366	1.145	19.694	1.00 30.56	A
	MOTA	2234	CG	GLN	Α	352	33.169	0.041	19.041	1.00 30.88	A
35	ATOM	2235	CD	GLN	A	352	34.493	-0.186	19.729	1.00 31.21	A
	ATOM	2236	OE1	GLN	A	352	34.541	-0.450	20.928	1.00 30.76	· A .
	MOTA	2237	NE2	GLN	A	352	35.578	-0.084	18.971	1.00 32.30	A
	ATOM	2238	C			352	30.504	2.638	18.963	1.00 30.42	A
	ATOM	2239	0			352	29.595	1.831	18.770	1.00 29.01	A
40	MOTA	2240	N			353	30.290	3.875	19.397	1.00 27.64	A
	MOTA	2241	CA			353	28.948	4.365	19.652	1.00 27.42	A A
	MOTA	2242	CB			353	28.977	5.401	20.775	1.00 25.77 1.00 27.34	A
	ATOM	2243	CG			353	29.408	4.837 5.914	22.115 23.156	1.00 27.34	A
	ATOM	2244	CD			353	29.638	6.872	23.150	1.00 27.15	A
45	ATOM	2245		GLN			28.875 30.687	5.753	23.252	1.00 28.79	A
	ATOM	.2246		GLN				4.989	18.385	1.00 29.00	A
	MOTA	2247	C			353	29.118	5.455	17.516	1.00 29.14	A
	ATOM	2248	0			353 354		4.984	18.276	1.00 27.31	A
50	MOTA	2249 2250	N CA			354		5.568	17.119	1.00 27.85	A
50	ATOM ATOM	2251	CB			354		4.941	16.904	1.00 30.69	A
	ATOM	2251		THR				3.532	16.665	1.00 30.07	A
	ATOM	2252		THR				5.585	15.709	1.00 29.58	A
	ATOM	2254	.C			354		7.062	17.376	1.00 26.85	A
55	ATOM	2255	0			354		7.475	18.329	1.00 25.77	A
0.5	ATOM	2256	N			355		7.898	16.533	1.00 27.22	A
	ATOM	2257	CD			355		7.588	15.431	1.00 25.89	
	ATOM	2258	CA			355		9.346	16.734	1.00 27.23	A
	ATOM	2259	CB			355		9.915	15.609	1.00 24.91	Α

	ATOM	2260	CG	PRO	A	355		28.643	8.838	15.385	1.00	25.54	٠,	A
	ATOM	2261	С	PRO	Α	355		25.322	9.837	16.641	1.00	28.07		A
	MOTA	2262	ō	PRO				24.548	9.364	15.810		27.24		Α
	ATOM	2263	N	PRO				24.941	10.792	17.500	1.00	28.28	٠.	Α
5	ATOM	2264	CD	PRO				25.752	11.560	18.462		28.31		A
J	ATOM	2265	CA	PRO				23.572	11.306	17.448		28.44		Α
		2266	CB	PRO				23.539	12.301	18.604		28.11		A
	ATOM			PRO				24.946	12.832	18.612		26.86		A
	ATOM	2267	CG	PRO				23.363	11.978	16.012		29.25		A
10	MOTA	2268	C	PRO						15.529		27.27		Α
10	MOTA	2269	0					24.304	12.537					Α
	MOTA	2270	N	ALA				22.143	11.910	15.575		30.45		
	MOTA	2271	CA	ALA				21.848	12.521	14.287	_	32.81		A
	ATOM	2272	CB	ALA				20.507	12.019	13.757		31.99		A
	ATOM	2273	С	ALA	Α	357		21.824	14.035	14.448		35.05		A
15	MOTA	2274	0	ALA				21.194	14.561	15.369		35.04		A
	MOTA	2275	N	LEU	Α	358		22.516	14.730	13.552		37.81		A
	ATOM	2276	CA	LEU	Α	358		22.578	16.185	13.597		42.15		A
	MOTA	2277	CB	LEU	Α	358		23.679	16.681	12.658	1.00	39.54		Α
	ATOM	2278	CG	LEU	A	358		25.086	16.285	13.109	1.00	39.51		A
20	ATOM	2279	CD1	LEU	Α	358		26.102	16.686	12.062	1.00	39.29		A
	ATOM	2280	CD2	LEU	Α	358		25.395	16.953	14.445	1.00	40.01		Α
	ATOM	2281	С	LEU	Α	358		21.241	16.837	13.242	1.00	45.91		A
	ATOM	2282	.0	LEU				20.874	16.927	12.069	1.00	45.71		Α
	ATOM	2283	N			359		20.530	17.290	14.275	1.00	50.06		A
25	ATOM	2284	CA	THR				19.223	17.939	14.140	1.00	53.73		Α
23	ATOM	2285	CB	THR				19.353	19.428	13.726		54.04		A
		2286		THR				19.995	19.521	12.448		56.35		A
	ATOM			THR				20.158	20.204	14.763		54.32		Α
	ATOM	2287				359		18.309	17.236	13.139		54.47		Α
20	ATOM	2288	C						16.016	12.930		55.90	-	A
30	MOTA	2289	0			359		18.483	17.908	12.595		56.97		A
	MOTA	2290	OXT	THR	A	359		17.407	17.508	12.333	1.00	50.57	•	•
	TER	_			_			00 020	54 646	-7.659	1 00	20.00	6	
	MOTA	. 1	CB	PRO		71		99.838	54.646			20.00	6	
	ATOM	2	CG	PRO		71		99.216	55.105	-6.341			6	
35	MOTA	3	C	PRO		71		98.903	54.776	-9.981		20.00	8	
	MOTA	4	0	PRO				98.022		-10.109		20.00		
	MOTA	5	И	PRO				97.782	55.851	-8.042		20.00	7	
	MOTA	6	CD	PRO	В			97.728	55.323	-6.668		20.00	6	
	MOTA	7	CA	PRO			٠	99.087	55.515	-8.658		20.00	6	
40	MOTA	8	N	PRO	В			99.732		-10.985		20.00	7	
	MOTA	9	CD	PRO	В	72		100.794		-10.977		20.00	6	
	MOTA	· 10	CA	PRO	В	72		99.645		-12.297		20.00	6	
	ATOM	11	CB	PRO	В	72		100.885		-13.017		20.00	6	
	ATOM	12	CĠ	PRO	В			101.026		-12.456		20.00	6	
45	MOTA	13	C	PRO	В	72		99.627	52.924	-12.202		20.00	6	
	ATOM	14	0	PRO	В	72		100.246	52.338	-11.314	1.00	20.00	8	
	ATOM	15	N	ALA	В	73		98.906	52.293	-13.122		20.00	7	
	ATOM	16	CA	ALA	В	73		98.805	50.840	-13.167	1.00	20.00	6	
	ATOM	17	CB	ALA				97.420	50.392	-12.710	1.00	20.00	6	
50	ATOM	18	C	ALA				99.053	50.398	-14.604	1.00	20.00	6	
50	ATOM	19	0	ALA				99.027	51.215	-15.526	1.00	20.00	8	
	MOTA	20	N	PRO				99.313		-14.818	1.00	20.00	7	
	ATOM	21	CD	PRO				99.473		-13.857		20.00	6	
	ATOM	22	CA	PRO				99.553		-16.189		20.00	6	
55		23	CB	PRO				99.700		-16.023		20.00	6 -	
JJ	ATOM		CG	PRO				100.292		-14.649		20.00	6	
	ATOM	24	C	PRO				98.371		-17.079		20.00	6	
	ATOM	25		PRO				97.279		-16.583		20.00	8	
	ATOM	26	0							-18.389		20.00	7.	
	MOTA	27	N	ALA	В	75		98.589	42.03/	-10.303	1.00	20.00	•	

	ATOM	28	CA	ALA :	В	75	97.516	49.368 -19.321 1.00 20.00	6
	ATOM	29	CB	ALA	В	75	98.061	49.462 -20.745 1.00 20.00	6
	ATOM	30	С	ALA :	В	75	96.446	48.285 -19.246 1.00 20.00	6
	ATOM	31	0	ALA :	В	75	96.745	47.126 -18.961 1.00 20.00	8
5	ATOM	32	N	LYS :	В	76	95.200	48.666 -19.494 1.00 20.00	7
	ATOM	33	CA	LYS	В	76	94.098	47.716 -19.463 1.00 20.00	6
	ATOM	34	CB	LYS :	В	76	92.793	48.431 -19.805 1.00 20.00	
	ATOM	35	CG	LYS	В	76	91.546	47.792 -19.225 1.00 20.00	
	ATOM	36	CD	LYS	В	76	91.511	47.932 -17.711 1.00 20.00	
10	ATOM	37	CE	LYS	В	76	90.184	47.454 -17.152 1.00 20.00	
	MOTA	38	NZ	LYS	В	76	90.108	47.606 -15.673 1.00 20.00	
	ATOM	39	С	LYS	В	76	94.389	46.645 -20.513 1.00 20.00	
	ATOM	40	0	LYS	В	76	94.736	46.968 -21.645 1.00 20.00	
	ATOM	41	N	LYS	В	77	94.269	45.374 -20.145 1.00 20.00	
15	ATOM	42	CA	LYS	В	77	94.525	44.311 -21.107 1.00 20.00	
	MOTA	43	CB	LYS	В	77	94.875	43.008 -20.384 1.00 20.00	
	ATOM	44	CG	LYS	В	77	96.117	43.125 -19.506 1.00 20.00	
	MOTA	45	CD	LYS	В	77	96.461	41.812 -18.842 1.00 20.00	
	MOTA	46	CE	LYS		77	97.501	42.008 -17.745 1.00 20.00	
20	MOTA	47	NZ	LYS	В	77	98.771	42.582 -18.255 1.00 20.00	
	MOTA	48	C	LYS	В	77	93.311	44.111 -22.012 1.00 20.00	
	ATOM	49	0	LYS	В	7.7	92.218	44.585 -21.704 1.00 20.00	
	MOTA	50	N	ARG		78	93.514	43.418 -23.129 1.00 20.00	
_	ATOM	51	CA	ARG	В	78	92.442	43.158 -24.086 1.00 20.00	
25	ATOM	52	CB	ARG	В	78	92.465	44.224 -25.193 1.00 20.00	
	ATOM	53	CG	ARG		78	93.787	44.344 -25.925 1.00 20.00	
	MOTA	54	CD	ARG		78	93.833	45.612 -26.771 1.00 20.00	
	ATOM	55	NE	ARG		78	95.052	45.702 -27.575 1.00 20.00	-
	MOTA	56	CZ	ARG		78	96.287	45.751 -27.078 1.00 20.00	
30	MOTA	57		ARG		78	96.486	45.721 -25.764 1.00 20.00	
	MOTA	58		ARG		78	97.330	45.828 -27.897 1.00 20.00	
	MOTA	59	С	ARG		78	92.570	41.754 -24.678 1.00 20.00 41.126 -24.581 1.00 20.00	
	MOTA	60	0	ARG		78	93.625		
	MOTA	61	N	PRO		79	91.494		
35	MOTA	62	CD	PRO		79 	90.195		
	MOTA	63	CA	PRO		79	91.519	39.899 -25.896 1.00 20.00 39.848 -26.691 1.00 20.00	
	MOTA	64	CB	PRO		79	90.214	40.725 -25.889 1.00 20.0	_
	ATOM	65	CG	PRO		79	89.304	39.614 -26.778 1.00 20.0	
	MOTA	66	C	PRO		79 70	92.737 93.311	38.523 -26.717 1.00 20.0	
40	MOTA	67	0	PRO		79	93.311	40.597 -27.589 1.00 20.0	
	ATOM	68	N	GLU		80 80	94.254	40.441 -28.503 1.00 20.0	_
	MOTA	69	CA	GLU			94.358	41.644 -29.446 1.00 20.0	
	ATOM	70	CB			80	94.330	42.912 -28.800 1.00 20.0	_
	MOTA	71	CG	GLU		80	95.009	44.057 -29.788 1.00 20.0	
45	ATOM	72	CD	GLU		80 80	93.968	44.513 -30.308 1.00 20.0	
	MOTA	73		GLU			96.150	44.498 -30.047 1.00 20.0	
	MOTA	74		GLU		80	95.591	40.235 -27.787 1.00 20.0	
	ATOM	75	C	GLU		80 80	96.558	39.795 -28.405 1.00 20.0	
50	ATOM	76	O	ASP		81	95.656	40.559 -26.497 1.00 20.0	
50	MOTA	77	N CA	ASP		81	96.902	40.380 -25.749 1.00 20.0	
	ATOM	78	CB	ASP		81	96.888	41.192 -24.446 1.00 20.0	
	ATOM	79 80	CG	ASP		81	96.774	42.688 -24.682 1.00 20.0	
	MOTA	80		ASP		81	97.436	43.193 -25.606 1.00 20.0	
<i>E E</i>	MOTA	81 82		ASP		81	96.033	43.362 -23.933 1.00 20.0	
55	ATOM		C	ASP		81	97.111	38.914 -25.393 1.00 20.0	
	MOTA	83 84	0	ASP		81	98.172	38.535 -24.890 1.00 20.0	
	ATOM	84 85	N	PHE		82	96.103	38.093 -25.679 1.00 20.0	
	ATOM	86	CA	PHE		82	96.140	36.677 -25.340 1.00 20.0	
	ATOM	.00	CA	* 1113		02			

	ATOM	87	CB	PHE	В	82	95.056	36.369 -24.302	1.00 20.00	6
	MOTA	88	CG	PHE	В	82	95.157	37.187 -23.050	1.00 20.00	6
	MOTA	89	CD1	PHE	В	82	95.880	36.724 -21.959	1.00 20.00	6
	ATOM	90	CD2	PHE	В	82	94.525	38.423 -22.961	1.00 20.00	6
5	ATOM	91	CE1	PHE	В	82	95.976	37.479 -20.793	1.00 20.00	6
	ATOM	92	CE2	PHE	В	82	94.615	39.188 -21.800	1.00 20.00	6
	ATOM	93	CZ	PHE	В	82	95.343	38.712 -20.713	1.00 20.00	6
	MOTA	94	C	PHE	В	82	95.929	35.719 -26.496	1.00 20.00	6
	ATOM	95	0	PHE	В	82	95.342	36.061 -27.524	1.00 20.00	8
10	ATOM	96	N	LYS	В	83	96.406	34.500 -26.286	1.00 20.00	7
	MOTA	97	CA	LYS	В	83	96.242	33.411 -27.228	1.00 20.00	6
	ATOM	98	CB	LYS	В	83	97.594	32.777 -27.562	1.00 20.00	6
	ATOM	99	CG	LYS	В	83	97.503	31.531 -28.425	1.00 20.00	6
	ATOM	100	CD	LYS	В	83	98.888	31.074 -28.856	1.00 20.00	6
15	ATOM	101	CE	LYS	В	83	98.826	29.808 -29.699	1.00 20.00	6
	ATOM	102	NZ	LYS	В	83	98.287	28.654 -28.918	1.00 20.00	7
	ATOM	103	C.	LYS	В	83	95.387	32.446 -26.416	1.00 20.00	6
	MOTA	104	0	LYS	В	83	95.884	31.776 -25.510	1.00 20.00	8
	ATOM	105	N	PHE	В	84	94.094	32.393 -26.710	1.00 20.00	7
20	ATOM	106	CA	PHE	В	84	93.217	31.511 -25.958	1.00 20.00	6
	ATOM	107	CB	PHE	В	84	91.758	31.928 -26.133	1.00 20.00	6
	ATOM	108	CG	PHE	В	84	91.426	33.228 -25.462	1.00 20.00	6
	MOTA	109	CD1	PHE	В	84	91.668	34.439 -26.099	1.00 20.00	6
	ATOM	110	CD2	PHE	В	84	90.907	33.243 -24.174	1.00 20.00	6
25	ATOM	111	CE1	PHE	В	84	91.400	35.644 -25.464	1.00 20.00	6
	MOTA	112	CE2	PHE	В	84	90.636	34.447 -23.528	1.00 20.00	6
	ATOM	113	cz	PHE	В	84	90.884	35.646 -24.176	1.00 20.00	6
	ATOM	114	С	PHE	В	84	93.402	30.054 -26.335	1.00 20.00	6
	ATOM	115	0	PHE	В	84	93.734	29.734 -27.476	1.00 20.00	8
30	MOTA	116	N	GLY	В	85	93.196	29.178 -25.359	1.00 20.00	7
	ATOM	117	CA	GLY	В	85	93.349	27.758 -25.591	1.00 20.00	6
	MOTA	118	C	GLY	В	85	92.103	26.977 -25.221	1.00 20.00	6
	ATOM	119	0	GLY	В	85	90.982	27.393 -25.525	1.00 20.00	8
	MOTA	120	N	LYS	В	86	92.296	25.858 -24.534	1.00 20.00	7
35	MOTA	121	CA	LYS	В	86	91.182	25.005 -24.153	1.00 20.00	6
	ATOM	122	CB	LYS	В	86	91.695	23.640 -23.687	1.00 20.00	6
	MOTA	123	CG	LYS	В	86	92.421	23.667 -22.356	1.00 20.00	6
	MOTA	124	CD	LYS	В	86	92.855	22.272 -21.941	1.00 20.00	6
	MOTA	125	CE	LYS	В	86	93.685	22.319 -20.668	1.00 20.00	6 7
40	MOTA	126	NZ	LYS		86	94.209	20.975 -20.287	1.00 20.00	
	ATOM	127	C	LYS		86	90.267	25.576 -23.077	1.00 20.00	6
	MOTA	128	0	LYS		86	90.668	26.410 -22.260	1.00 20.00	8 7
	MOTA	129	N	ILE		87	89.026	25.106 -23.102	1.00 20.00	
	ATOM	130	CA	ILE	В	87	88.023	25.497 -22.131	1.00 20.00	6
45	ATOM	131	CB	ILE		87	86.604	25.159 -22.647	1.00 20.00	6
	MOTA	132		ILE		87	85.582	25.261 -21.503	1.00 20.00	6
	MOTA	133		ILE		87	86.260	26.085 -23.820	1.00 20.00	6 6
	MOTA	134		ILE		87	84.912	25.819 -24.463	1.00 20.00	6
	MOTA	135	С	ILE		87	88.312	24.687 -20.872	1.00 20.00 1.00 20.00	8
50	MOTA	136	0	ILE		87	88.396	23.461 -20.927		7
	ATOM	137	N	LEU		88	88.473	25.368 -19.742	1.00 20.00 1.00 20.00	6
	MOTA	138	CA	LEU		88	88.757	24.686 -18.486	1.00 20.00	6
	MOTA	139	СВ	LEU		88	89.592	25.586 -17.575	1.00 20.00	6
	MOTA	140	CG	LEU		88	90.968	25.987 -18.112	1.00 20.00	6
55	MOTA	141		LEU		88	91.611	27.006 -17.186	1.00 20.00	6
	MOTA	142		LEU		88	91.836	24.756 -18.234	1.00 20.00	6
	ATOM	143	C	LEU		88	87.471	24,298 -17.776	1.00 20.00	8
	MOTA	144	0	LEU		88	87.434	23.334 -17.014	1.00 20.00	7
	MOTA	145	N	GLY	В	89	86.410	25.051 -18.024	1.00 20.00	,

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	MOTA	146	CA .	GLY	В	89	85.148	24.749 -17.382	1.00 20.00	6
	ATOM	147	С	GLY	В	89	84.038	25.599 -17.953	1.00 20.00	6
	ATOM	148	0	GLY	В	89	84.296	26.657 -18.541	1.00 20.00	8
	MOTA	149	N	GLU	В	90	82.807	25.133 -17.781	1.00 20.00	7
5	MOTA	150	CA	GLU	В	90	81.629	25.832 -18.279	1.00 20.00	6
	ATOM	151	CB	GLU	В	90	81.041	25.070 -19.471	1.00 20.00	6
	MOTA	152	CG	GLU	В	90	81.929	25.084 -20.706	1.00 20.00	6
	MOTA	153	CD	GLU	В	90	81.434	24.157 -21.802	1.00 20.00	6
	ATOM	154	OE1	GLU	В	90	81.539	22.923 -21.639	1.00 20.00	8
10	MOTA	155	OE2	GLU		90	80.935	24.662 -22.827	1.00 20.00	8
	ATOM	156	C	GLU	В	90	80.575	25.970 -17.188	1.00 20.00	6
	ATOM	157	0	GLU	В	90	80.208	24.994 -16.543	1.00 20.00	8
	ATOM	158	N	GLY	В	91	80.103	27.193 -16.979	1.00 20.00	7
	ATOM	159	CA	GLY	В	91	79.080	27.431 -15.979	1.00 20.00	6
15	ATOM	160	C	GLY	В	91	77.835	27.949 -16.673	1.00 20.00	6
	ATOM	161	0	GLY	В	91	77.804	28.046 -17.903	1.00 20.00	8
	ATOM	162	N	SER	В	92	76.808	28.291 -15.904	1.00 20.00	7
	ATOM	163	CA	SER	В	92	75.582	28.794 -16.508	1.00 20.00	6
	MOTA	164	CB	SER	В	92	74.428	28.719 -15.505	1.00 20.00	6
20	ATOM	165	OG	SER	В	92	74.786	29.335 -14.282	1.00 20.00	8
	ATOM	166	C	SER	В	92	75.726	30.219 -17.039	1.00 20.00	6
	ATOM	167	0	SER	В	92	75.078	30.585 -18.018	1.00 20.00	8
	ATOM	168	N	PHE	В	93	76.578	31.025 -16.411	1.00 20.00	7
	ATOM	169	CA	PHE	В	93	76.763	32.399 -16.870	1.00 20.00	6
25	ATOM	170	CB	PHE	В	93	76.276	33.384 -15.807	1.00 20.00	6
	ATOM	171	CG	PHE	В	93	74.832	33.220 -15.469	1.00 20.00	6
	ATOM	172	CD1	PHE	В	93	74.435	32.323 -14.483	1.00 20.00	6
	ATOM	173	CD2	PHE	В	93	73.859	33.914 -16.183	1.00 20.00	6
	MOTA	174	CE1	PHE	В	93	73.086	32.117 -14.210	1.00 20.00	6
30	ATOM	175	CE2	PHE	В	93	72.507	33.715 ~15.919	1.00 20.00	- 6
	ATOM	176	CZ	PHE	В	93	72.120	32.812 -14.930	1.00 20.00	6
	ATOM	177	С	PHE	В	93	78.197	32.736 -17.240	1.00 20.00	6
	MOTA	178	0	PHE	В	93	78.543	33.908 -17.397	1.00 20.00	8
	ATOM	179	N	SER	В	94	79.030	31.713 -17.394	1.00 20.00	7
35	ATOM	180	CA	SER	В	94	80.421	31.948 -17.735	1.00 20.00	б
	ATOM ·	181	CB	SER	В	94	81.174	32.443 -16.503	1.00 20.00	6
	ATOM	182	OG	SER	В	94	81.237	31.410 -15.535	1.00 20.00	8
	MOTA	183	С	SER	В	94	81.123	30.707 -18.253	1.00 20.00	6
	ATOM	184	0	SER		94	80.666	29.584 -18.048	1.00 20.00	8
40	MOTA	185	N	THR		95	82.252	30.937 -18.913	1.00 20.00	7
	ATOM	186	CA	THR		95	83.088	29.879 -19.455	1.00 20.00	6
	ATOM	187	CB	THR		95	82.942	29.770 -20.985	1.00 20.00	6
	ATOM	188		THR		95	81.589	29.425 -21.309	1.00 20.00	8
	ATOM	189	CG2	THR	В	95	83.873	28.694 -21.536	1.00 20.00	6
45	ATOM	190	C	THR		95	84.524	30.264 -19.118	1.00 20.00	6
	ATOM	191	0	THR		95	84.957	31.388 ~19.399	1.00 20.00	8
	MOTA	192	N	VAL		96	85.257	29.348 -18.498	1.00 20.00	7
	ATOM	193	CA	VAL		96	86.642	29.628 -18.141	1.00 20.00	6
	ATOM	194	СВ	VAL		96	86.991	29.050 -16.761	1.00 20.00	6
50	ATOM	195		VAL		96	88.438	29.390 -16.407	1.00 20.00	6
	ATOM	196		VAL		96	86.041	29.627 -15.707	1.00 20.00	6
	ATOM	197	C	VAL		96	87.541	29.027 -19.210	1.00 20.00	6
	MOTA	198	ō	VAL		96	87.432	27.845 -19.540	1.00 20.00	8
	ATOM	199	N	VAL		97	88.416	29.858 -19.763	1.00 20.00	7
55	MOTA	200	CA	VAL		97	89.312	29.430 -20.824	1.00 20.00	6
	ATOM	201	CB	VAL		97	89.006	30.194 -22.130	1.00 20.00	6
	ATOM	202		VAL		97	89.828	29.624 -23.279	1.00 20.00	6
	ATOM	203		VAL		97	87.515	30.116 -22.444	1.00 20.00	6
	ATOM	204	C	VAL		97	90.771	29.664 -20.458	1.00 20.00	6
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	ATOM	205	0	VAL	В	97	91.122	30.698	-19.889	1.00 20.00	8
	ATOM	206	N	LEU	В	98	91.617	28.690	-20.770	1.00 20.00	7
	ATOM	207	CA	LEU	В	98	93.039		-20.499	1.00 20.00	6
	ATOM	208	CB	LEU		98	93.727		-20.618	1.00 20.00	6
5	ATOM	209	CG	LEU		98	95.240	27.421	-20.383	1.00 20.00	6
	ATOM	210	CD1	LEU	В	98	95.565	28.019	-19.021	1.00 20.00	6
	ATOM	211		LEU		98	95.739		-20.463	1.00 20.00	6
	ATOM	212	С	LEU	В	98	93.580		-21.552	1.00 20.00	6
	ATOM	213	0	LEU		98	93.293		-22.738	1.00 20.00	8
10	ATOM	214	N	ALA		99	94.343		-21.121	1.00 20.00	7
	ATOM	215	CA	ALA		99	94.897		-22.043	1.00 20.00	6
	ATOM	216	CB	ALA		99	94.087		-21.980	1.00 20.00	6
	ATOM	217	С	ALA		99	96.353		-21.723	1.00 20.00	6
	ATOM	218	0	ALA		99	96.748		-20.554	1.00 20.00	8
15	ATOM	219	N	ARG		100	97.152		-22.763	1.00 20.00	7
	ATOM	220	CA	ARG		100	98.554		-22.568	1.00 20.00	6
	MOTA	221	CB	ARG		100	99.442		-23.393	1.00 20.00	6
	ATOM	222	CG	ARG		100	100.934		-23.131	1.00 20.00	6
	ATOM	223	CD	ARG		100	101.770		-23.923	1.00 20.00	6
20	MOTA	224	NE	ARG			101.600		-23.469	1.00 20.00	7
	ATOM	225	CZ	ARG		100	102.059		-22.314	1.00 20.00	6
	ATOM	226		ARG			102.722		-21.473	1.00 20.00	7
	MOTA	227	NH2	ARG			101.864		-22.003	1.00 20.00	7
	MOTA	228	C	ARG		100	98.756		-23.004	1.00 20.00	6 8
25	MOTA	229	0	ARG		100	 98.454		-24.146	1.00 20.00	7
	ATOM	230	N	GLU		101	99.228		-22.087	1.00 20.00	6
	ATOM	231	CA	GLU			99.470		-22.408 -21.123	1.00 20.00	6
	ATOM	232	CB	GLU			99.709		-21.123	1.00 20.00	6
70	MOTA	233	CG	GLU		101.	99.986 100.164		-21.363	1.00 20.00	6
30	ATOM	234	CD	GLU		101	100.164		-19.114	1.00 20.00	8
	ATOM	235	OE1 OE2	GLU		101	99.765		-20.025	1.00 20.00	8
	MOTA	236 237	C	GLU			100.703		-23.317	1.00 20.00	6
	ATOM	237	0	GLU			101.773		-22.944	1.00 20.00	8
35	ATOM ATOM	239	N	PEA		102	100.546		-24.507	1.00 20.00	7
33	ATOM	240	CA	LEU			101.632		-25.482	1.00 20.00	6
	ATOM	241	CB	LEU		102	101.145		-26.753	1.00 20.00	6
	ATOM	242	CG	LEU		102	100.013		-27.517	1.00 20.00	6
	ATOM	243		LEU		102	99.500		-28.623	1.00 20.00	6
40	MOTA	244		LEU		102	100.517		-28.089	1.00 20.00	6
-10	ATOM	245	C	LEU		102	102.906		-25.000	1.00 20.00	6
	MOTA	246	o	LEU			104.000		-25.180	1.00 20.00	8
	ATOM	247	N	ALA		103	102.760	38.828	-24.382	1.00 20.00	7
	ATOM	248	CA	ALA		103	103.909	39.587	-23.910	1.00 20.00	6
45	ATOM	249	CB	ALA			103.464	41.002	-23.546	1.00 20.00	6
	ATOM	250	C	ALA			104.697	38.983	-22.747	1.00 20.00	6
	ATOM	251	0	ALA	В	103	105.832	39.389	-22.503	1.00 20.00	8
	ATOM	252				104	104.122	38.007	-22.050	1.00 20.00	7
	ATOM		CA	THR	В	104	104.790	37.418	-20.893	1.00 20.00	6
50	MOTA	254	СВ	THR	В	104	104.059	37.799	-19.592	1.00 20.00	6
	ATOM	255	OG1	THR	В	104	102.712	37.303	-19.648	1.00 20.00	
	ATOM	256	CG2	THR	В	104	104.033	39.313	-19.404	1.00 20.00	
	MOTA	257	C	THR	В	104	104.880		-20.901	1.00 20.00	6
	ATOM	258	0	THR	В	104	105.677		-20.160	1.00 20.00	
55	MOTA	259	N	SER	В	105	104.042		-21.722	1.00 20.00	
	MOTA	260	CA	SER	В	105	103.950		-21.842	1.00 20.00	6
	ATOM	261	CB			105	105.344		-22.048	1.00 20.00	
	ATOM	262	OG			105	105.264		-22.287	1.00 20.00	
	MOTA	263	С	SER	В	105	103.304	33.243	-20.576	1.00 20.00	6

	ATOM	264	0	SER I	3 105	103.286	32.029 -20.363	1.00 20.00	8
	MOTA	265	N	ARG I	3 106	102.771	34.124 -19.736	1.00 20.00	7
	ATOM	266	CA	ARG 1	3 106	102.089	33.709 -18.509	1.00 20.00	6
	ATOM	267	CB	ARG I	3 106	101.833	34.914 -17.598	1.00 20.00	6
5	MOTA	268	CG	ARG I	3 106	103.022	35.361 -16.781	1.00 20.00	6
•	ATOM	269	CD	ARG 1	3 106	102.724	36.653 -16.045	1.00 20.00	6
	ATOM	270	NE	ARG I	B 106	103.756	36.940 -15.051	1.00 20.00	7
	ATOM	271	CZ		B 106	103.964	38.132 -14.504	1.00 20.00	6
	ATOM	272			B 106	103.210	39.167 -14.858	1.00 20.00	7
10	MOTA	273			B 106	104.918	38.279 -13.590	1.00 20.00	7
10	ATOM	274	C		В 106	100.743	33.082 -18.856	1.00 20.00	6
	MOTA	275	0		B 106	100.069	33.534 -19.777	1.00 20.00	8
	ATOM	276	N		B 107		32.049 ~18.115	1.00 20.00	7
	ATOM	277	CA		B 107	99.072	31.390 -18.336	1.00 20.00	6
15		278	CB		B 107		29.870 -18.212	1.00 20.00	6
15	MOTA	279	CG		B 107		29.207 -19.144	1.00 20.00	6
	MOTA	280	CD	GLU			27.696 -19.023	1.00 20.00	6
	· MOTA ·			GLU :			27.068 -19.798	1.00 20.00	8
	MOTA	281		GLU			27.144 -18.138	1.00 20.00	8
	ATOM	282					31.848 -17.285	1.00 20.00	6
20	MOTA	283	C		B 107		31.833 -16.095	1.00 20.00	8
	MOTA	284	0		B 107		32.243 -17.727	1.00 20.00	7
	MOTA	285	N		B 108		32.667 -16.817	1.00 20.00	6
	MOTA	286	CA	TYR			34.156 -16.979	1.00 20.00	6
	MOTA	287	CB	TYR			35.089 -16.487	1.00 20.00	6
25	MOTA	288	CG		B 108		35.369 -15.129	1.00 20.00	6
	ATOM	289			B 108		36.260 -14.674	1.00 20.00	6
	MOTA	290			B 108 B 108		35.712 -17.386	1.00 20.00	6
	MOTA	291	CD2				36.597 -16.950	1.00 20.00	6
	MOTA	292	CE2		B 108		36.869 -15.599	1.00 20.00	6
30	MOTA	293	CZ		B 108		37.756 -15.187	1.00 20.00	8
	MOTA	294	ОН				31.899 -17.167	1.00 20.00	6
	MOTA	295	C		B 108		31.463 -18.306	1.00 20.00	8
	MOTA	296	0		B 108		31.723 -16.181	1.00 20.00	7
	MOTA	297	N		B 109		31.073 -16.414	1.00 20.00	6
35	MOTA	298	CA		B 109		30.225 -15.214	1.00 20.00	6
	ATOM	299	CB	ALA			32.288 -16.542	1.00 20.00	6
	ATOM	300	C		B 109		33.003 -15.558	1.00 20.00	8
	ATOM	301	0	ILE			32.557 -17.756	1.00 20.00	7
	MOTA	302	N			_	33.711 -17.968	1.00 20.00	6
40	ATOM	303	CA	ILE			34.462 -19.271	1.00 20.00	6
	ATOM	304	CB				35.630 -19.507	1.00 20.00	6
	ATOM	305	CG2		B 110		34.962 -19.159	1.00 20.00	6
	MOTA	306			B 110		35.847 -20.312	1.00 20.00	б
	ATOM	307					•	1.00 20.00	6
45	ATOM	308	C		B 11		32.527 -18.851	1.00 20.00	8
	ATOM	309			B 11		33.852 -17.052	1.00 20.00	7
	ATOM	310	N	LYS	B 11		33.581 -16.975	1.00 20.00	6
	ATOM	311	CA		B 11		33.721 -15.531	1.00 20.00	6
	ATOM	312	CB		B 11		33.598 -15.411	1.00 20.00	6
50	ATOM	313	CG		B 11		33.590 -13.965	1.00 20.00	6
	MOTA	314	CD		B 11		32.262 -13.277	1.00 20.00	6
	ATOM	315	CE		B 11		32.202 -13.277	1.00 20.00	7
	ATOM	316	NZ		B 11		34.601 -17.869	1.00 20.00	6
	ATOM	317	C		B 11			1.00 20.00	8
55	ATOM	318	0	TITE	B 11 B 11	2 85.078		1.00 20.00	7
	MOTA	319			B 11			1.00 20.00	6
	MOTA	320		TT TO	B 11	2 84.695		1.00 20.00	6
	MOTA	321						1.00 20.00	6
	MOTA	322	CG	2 ILE	D TT	2 07.072	33.303 -44.210		

	ATOM	323	CG1	ILE E	3 112	86.216	34.518 -21.440	1.00 20.00	6
	MOTA	324	CD1	ILE E	3 112	86.657	33.949 -22.779	1.00 20.00	6
	ATOM	325	C	ILE E	3 112	82.878	34.916 ~19.538	1.00 20.00	6
	MOTA	326	0	ILE E	3 112	82.288	33.839 -19.510	1.00 20.00	8
5	ATOM	327	N	LEU I	3 113	82.269	36.083 -19.347	1.00 20.00	7
	ATOM	328	CA	LEU I	3 113	80.835	36.172 -19.089	1.00 20.00	6
	ATOM	329	CB	LEU I	3 113	80.585	36.696 -17.669	1.00 20.00	6
	ATOM	330	CG	LEU I	B 113	81.350	36.038 -16.521	1.00 20.00	6
	ATOM	331	CD1	LEU I	B 113	82.743	36.638 -16.428	1.00 20.00	6
10	ATOM	332	CD2	LEU I	B 113	80.609	36.258 -15.215	1.00 20.00	6
	MOTA	333	С	PEA 1	B 113	80.172	37.110 -20.090	1.00 20.00	6
	MOTA	334	0	LEU 1	B 113	80.634	38.232 -20.299	1.00 20.00	8
	MOTA	335	N	GLU I	B 114	79.088	36.653 -20.709	1.00 20.00	7
	MOTA	336	CA	GLU I	B 114	78.377	37.472 -21.681	1.00 20.00	6
15	ATOM	337	CB	GLU I	B 114	77.514	36.586 -22.581	1.00 20.00	6
	ATOM	338	CG	GLU 1	B 114	76.670	37.366 -23.571	1.00 20.00	6
	MOTA	. 339	CD ·	GLU I	B 114	75.749	36.473 -24.372	1.00 20.00	6
	MOTA	340	OE1	GLU I	B 114	75.083	35.613 -23.760	1.00 20.00	8
	MOTA	341	OE2	GLU :	B 114	75.684	36.638 -25.611	1.00 20.00	8
20	ATOM	342	C .	GLU :	B 114	77.509	38.491 -20.942	1.00 20.00	6
	ATOM	343	0	GLU :	B 114	76.673	38.122 -20.113	1.00 20.00	8
	ATOM	344	N	LYS :	B 115	77.709	39.771 -21.235	1.00 20.00	7
	ATOM	345	CA	LYS :	B 115	76.945	40.808 -20.553	1.00 20.00	6
	MOTA	346	CB	LYS :	B 115	77.433	42.202 -20.978	1.00 20.00	6
25	ATOM	347	CG	LYS	B 115	78.653	42.675 -20.183	1.00 20.00	6
	MOTA	348	CD	LYS	B 115	79.174	44.045 -20.618	1.00 20.00	6
	MOTA	349	CE	LYS	B 115	79.832	43.994 -21.992	1.00 20.00	6
	MOTA	350	NZ	LYS	B 115	80.536	45.273 -22.323	1.00 20.00	7
	ATOM	351	C	LYS.	B 115	75.435	40.693 -20.743	1.00 20.00	6
30	MOTA	352	0	LYS	B 115	74.676	40.787 -19.778	1.00 20.00	8
	MOTA	353	и.	ARG	B 116	74.997	40.471 -21.977	1.00 20.00	7
	MOTA	354	CA	ARG	B 116	73.570	40.363 -22.255	1.00 20.00	6
	MOTA	355	CB	ARG	B 116	73.346	40.066 -23.743	1.00 20.00	. 6
	MOTA	356	CG	ARG	B 116	71.893	39.821 -24.142	1.00 20.00	6
35	ATOM	357	CD		B 116	70.931	40.791 -23.465	1.00 20.00	6 7
	MOTA	358	NE		B 116	71.401	42.172 -23.493	1.00 20.00	6
	ATOM	35 <i>9</i>	CZ	ARG		70.780	43.177 -22.884	1.00 20.00	7
	MOTA	360			B 116	69.663	42.949 -22.207	1.00 20.00	7
	MOTA	361			B 116	71.278	44.405 -22.942	_	6
40	MOTA	362	С		B 116	72.888	39.298 -21.394	1.00 20.00	8
	MOTA	363	0		B 116	71.862	39.567 -20.764		7
	MOTA	364	N		B 117	73.463	38.101 -21.347		6
	MOTA	365	CA	HIS		72.885	37.020 -20.556		6
	ATOM	366	CB		B 117	73.704	35.738 -20.723 34.525 -20.133		6
45	MOTA	367	CG		B 117	73.053			6
	MOTA	368			B 117	71.762	34.274 -19.810		7
	MOTA	369			B 117	73.752	33.376 -19.836		6
	ATOM -	370			B 117	72.921	32.467 -19.355		7
	ATOM	371			B 117	71.707	32.987 -19.330 37.386 -19.077		6
50	MOTA	372	C		B 117	72.816	37.113 -18.409		8
	ATOM	373	0		B 117	71.823	37.992 -18.564		7
	ATOM	374	N		B 118	73.882	38.391 -17.160		6
	ATOM	375	CA		B 118 B 118	73.927 75.269	39.073 -16.827		6
	ATOM	376	CB		B 118	75.269	39.787 -15.486		6
55	MOTA	377	CG2		B 118	76.392	38.029 -16.834		6
	MOTA	378			B 118	77.784			6
	. ATOM	379			B 118		39.353 -16.833		6
	ATOM	380	C		B 118				8
	MOTA	381	0	TUE	0	, 2 . 1 0 1			

	MOTA	382	N	ILE	В	119		72.596	40.349	-17.690	1.00	20.00	7
	MOTA	383	CA	ILE	В	119		71.538	41.333	-17.494	1.00	20.00	6
	ATOM	384	CB	ILE	В	119		71.646	42.473	-18.539	1.00	20.00	6
	ATOM	385	CG2	ILE	В	119		70.396	43.357	-18.492	1.00	20.00	6
5	ATOM	386	CG1	ILE	В	119		72.919	43.292	-18.270	1.00	20.00	6
	MOTA	387	CD1	ILE	В	119		73.212	44.370	-19.314	1.00	20.00	6
	ATOM	388	C	ILE	В	119	•	70.154	40.687	-17.580	1.00	20.00	6
	ATOM	389	0	ILE	В	119	-	69.289	40.953	-16.747	1.00	20.00	8
	ATOM	390	N	LYS	В	120		69.950	39.832	-18.579		20.00	7
10	ATOM	391	CA	LYS	В	120		68.659		-18.754	1.00	20.00	6
	MOTA	392	CB	LYS	В	120		68.697	38.200	-19.935	1.00	20.00	6
	ATOM	393	CG	LYS	В	120		68.942	38.841	-21.284	1.00	20.00	6
	ATOM	394	CD	LYS	В	120		68.926	37.782	-22.387	1.00	20.00	6
	ATOM	395	CE	LYS	В	120		69.934	36.665	-22.093	1.00	20.00	6
15	ATOM	396	NZ	LYS	В	120		69.950	35.599	-23.127	1.00	20.00	7
	ATOM	397	C	LYS	В	120		68.229	38.398	-17.513	1.00	20.00	6
	ATOM	398	0	LYS	В	120		67.077	38.490	-17.092	1.00	20.00	8
	ATOM	399	N.	GLU	В	121		69.154	37.639	-16.930	1.00	20.00	7
	ATOM	400	CA	GLU	В	121		68.851	36.839	-15.747	1.00	20.00	6
20	ATOM	401	CB	GLU	В	121		69.678	35.549	-15.758		20.00	6
	MOTA	402	CG	GLU	В	121		69.485	34.674	-16.995	1.00	20.00	6
	ATOM	403	CD	GLU	В	121		68.029	34.326	-17.248		20.00	6
	MOTA	404	OE1	GLU	В	121		67.339	33.904	-16.295		20.00	8
	ATOM	405	OE2	GLU	В	121		67.574		-18.404		20.00	8
25	ATOM	406	С	GLU	В	121		69.071	37.573	-14.424		20.00	6
	ATOM	407	0	GLU	В	121		69.117	36.946	-13.362		20.00	8
	ATOM	408	N	ASN	В	122		69.208	38.895	-14.485	1.00	20.00	7
	MOTA	409	CA	ASN	В	122		69.411	39.699	-13.281		20.00	6
	MOTA	410	CB	ASN	В	122		68.132		-12.439		20.00	6
30	ATOM	411	CG	ASN	В	122		66.952		-13.177		20.00	6
	ATOM	412	OD1	ASN	В	122		66.428		-14.121		20.00	8
	ATOM	413	ND2	ASN	В	122		66.530	41.498	-12.748		20.00	7
	ATOM	414	С	ASN	В	122		70.563		-12.419		20.00	6
	ATOM	415	0	ASN	В	122		70.408	39.007	-11.212		20.00	8
35	ATOM	416	N	LYS	В	123		71.716		-13.033		20.00	7
	ATOM	417	CA	LYS	В	123		72.870		-12.301		20.00	6
	ATOM	418	CB	LYS	В	123		73.500		-13.065		20.00	6
	ATOM	419	CG	LYS	В	123		72.568		-13.276		20.00	6
	ATOM	420	CD	LYS	В	123		72.065		-11.948		20.00	6
40	ATOM	421	CE	LYS	В	123		71.032		~12.159		20.00	6
	ATOM	422	NZ	LYS	В	123		70.421		-10.871		20.00	7
•	ATOM	423	С	LYS	В	123		73.931	39.498	-12.054		20.00	6
	ATOM	424	0.	$rac{r}{\lambda}$	В	123		75.035	39.183			20.00	8
	ATOM	425	N	VAL	В	124		73.607		-12.340			7
45	ATOM	426	CA	VAL	В	124		74.575		-12.145		20.00	6
	ATOM	427	CB	VAL	В	124		73.997		-12.547		20.00	6
	ATOM	428	CG1	VAL	В	124		75.035		-12.302		20.00	6
	ATOM	429	CG2	VAL	В	124		73.608		-14.022		20.00	6
	MOTA	430	C	VAL	В	124		75.091		-10.712		20.00	6
50 -	ATOM	431	0	VAL	В	124		76.278		-10.490		20.00	8
	MOTA	432	N			125		74.207	41.695	-9.716		20.00	7
	MOTA	433	CD			125		72.735	41.613	-9.757		20.00	6
	MOTA	434	CA			125		74.688	41.747	-8.331		20.00	6
	MOTA	435	CB			125		73.411	41.558	-7.512		20.00	6
55	ATOM	436	CG			125		72.346	42.152	-8.396		20.00	6
	ATOM	437	С			125		75.715	40.643	-8.051		20.00	6
	MOTA	438	0			125		76.683	40.851	-7.325		20.00	8
	ATOM	439	N			126		75.493	39.475	-8.640		20.00	7
	ATOM	440	CA	TYR	В	126		76.380	38.334	-8.440	1.00	20.00	6

	MOTA	441	CB	TYR	В	126	75.699	37.059	-8.942	1.00 20.00	б
	ATOM	442	CG	TYR	В	126	74.479	36.687	-8.127	1.00 20.00	6
	MOTA	443	CD1	TYR	В	126	74.611	36.068	-6.884	1.00 20.00	6
-	MOTA	444	CE1	TYR	В	126	73.491	35.748	-6.112	1.00 20.00	6
5	ATOM	445	CD2	TYR	В	126	73.193	36.981	-8.583	1.00 20.00	6
	ATOM	446	CE2	TYR	В	126	72.063	36.667	-7.817	1.00 20.00	6
	MOTA	447	CZ	TYR	В	126	72.223	36.052	-6.584	1.00 20.00	6
	ATOM	448	OH	TYR	В	126	71.118	35.743	-5.823	1.00 20.00	8
	ATOM	449	C	TYR	В	126	77.738	38.511	-9.113	1.00 20.00	6
10	ATOM	450	0	TYR	В	126	78.777	38.273	-8.492	1.00 20.00	8
	ATOM	451	N	VAL	В	127	77.738	38.931	-10.374	1.00 20.00	7
	ATOM	452	CA	VAL	В	127	78.994	39.123	-11.085	1.00 20.00	6
	ATOM	453	CB	VAL	В	127	78.756	39.466	-12.567	1.00 20.00	6
	ATOM	454	CG1	VAL	В	127	80.096	39.637	-13.275	1.00 20.00	6
15	ATOM	455	CG2	VAL	В	127	77.949		-13.234	1.00 20.00	6
	ATOM	456	С	VAL	В	127	79.798	40.242	-10.427	1.00 20.00	6
	ATOM	457	0	VAL	В	127	81.016 ·	40.148	-10.292	1.00 20.00	8
	ATOM	458	N	THR	В	128	79.105	41.293	-10.006	1.00 20.00	7
	ATOM	459	CA	THR			79.746	42.424	-9.345	1.00 20.00	6
20	ATOM	460	CB	THR	В	128	78.721	43.548	-9.070	1.00 20.00	6
	ATOM	461	OG1	THR	В	128	78.194	44.025	-10.316	1.00 20.00	8
	ATOM	462	CG2	THR	В	128	79.371	44.703	-8.330	1.00 20.00	6
	ATOM	463	С	THR	В	128	80.372	41.979	-8.019	1.00 20.00	6
	MOTA	464	0	THR	В	128	81.500	42.355	-7.696	1.00 20.00	8
25	ATOM	465	N	ARG	В	129	79.637	41.172	-7.256	1.00 20.00	7
	ATOM	466	CA	ARG	В	129	80.126	40.678	-5.971	1.00 20.00	6
	ATOM	467	CB	ARG	В	129	79.035	39.888	-5.254	1.00 20.00	6
	ATOM	468	CG	ARG	В	129	79.428	39.438	-3.852	1.00 20.00	6
	ATOM	469	CD	ARG	В	129	78.351	38.554	-3.278	1.00 20.00	6
30	MOTA	470	NE	ARG	В	129	77.048	39.209	-3.315	1.00 20.00	7
	ATOM	471	cz	ARG	В	129	75.894	38.569	-3.484	1.00 20.00	6
	MOTA	472	NH1	ARG	В	129	75.878	37.250	-3.636	1.00 20.00	7
	MOTA	473	NH2	ARG			74.756	39.248	-3.501	1.00 20.00	7
	MOTA	474	C	ARG	В	129	81.354	39.788	-6.146	1.00 20.00	6
35	MOTA	475	0	ARG	В	129	82.315	39.885	-5.379	1.00 20.00	8
	MOTA	476	N	GLU			81.316	38.917	-7.151	1.00 20.00	7
	MOTA	477	CA	GLU	В	130	82.439	38.029	-7.421	1.00 20.00	6
	MOTA	478	CB	$GL\Omega$			82.191	37.211	-8.692	1.00 20.00	6
	MOTA	479	CG	GLU			83.408	36.427	-9.167	1.00 20.00	6
40	MOTA	480	CD	GLU	В	130	83.060		-10.168	1.00 20.00	6
	MOTA	481		GLU		130	82.227		-11.061	1.00 20.00	8
	ATOM	482	OE2	GLU		130	83.626		-10.068	1.00 20.00	8
	ATOM	483	C	GLU		130	83.708	38.853	-7.580	1.00 20.00	6
	ATOM	484	0	GLU	В	130	84.723	38.575	-6.940	1.00 20.00	8
45	ATOM	485	N	ARG			83.641		-8.428	1.00 20.00	7
	ATOM	486	CA	ARG			84.788	40.742	-8.673	1.00 20.00	6
	MOTA	487	CB	ARG			84.459	41.759	-9.777	1.00 20.00	6
	ATOM	488	CG	ARG			85.580		-10.035	1.00 20.00	6
	ATOM	489	CD	ARG			85.262		-11.167	1.00 20.00	6
50	MOTA	490	NE	ARG			86.351		-11.355	1.00 20.00	. 7
	ATOM	491	CZ	ARG			86.416		-12.343	1.00 20.00	6
	MOTA	492		ARG			85.450		-13.250	1.00 20.00	7
	ATOM	493		ARG			87.450		-12.426	1.00 20.00	7
	ATOM	494	C			131	85.228	41.485	-7.409	1.00 20.00	6
55	MOTA	495	0	ARG			86.413	41.500	-7.071	1.00 20.00	8
	MOTA	496	N			132	84.277	42.103	-6.715		7 6
	MOTA	497	CA	ASP			84.594	42.848	-5.505	1.00 20.00	
•	MOTA	498	CB			132	83.350	43.575	-4.987	1.00 20.00	6 6
	MOTA	499	CG	ASP	В	132	82.865	44.658	-5.943	1.00 20.00	3

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	ATOM	500	OD1	ASP	В	132		83.612	45.010	-6.886	1.00	20.00	8
	ATOM	501	OD2	ASP	В	132	•	81.739	45.167	-5.747	1.00	20.00	8
	ATOM	502	C	ASP	В	132		85.192	41.969	-4.401	1.00	20.00	6
	ATOM	503	0	ASP	В	132		86.191	42.337	-3.783	1.00	20.00	8
5	ATOM	504	N	VAL	В	133		84.596	40.809	-4.150	1.00	20.00	7
	ATOM	505	CA	VAL	В	133		85.131	39.933	-3.116	1.00	20.00	6
	MOTA	506	CB	VAL	В	133		84.226	38.698	-2.885	1.00	20.00	6
•	ATOM	507	CG1	VAL	В	133		84.920	37.713	-1.957	1.00	20.00	6
	ATOM	508	CG2	VAL	В	133		82.893	39.135	-2.271	1.00	20.00	6
10	ATOM	509	С	VAL	В	133		86.540	39.470	-3.477	1.00	20.00	6
	ATOM	510	0	VAL	В	133		87.460	39.602	-2.675	1.00	20.00	8
	ATOM	511	N	MET	В	134		86.721	38.950	-4.688	1.00	20.00	7
	ATOM	5 1 2	CA	MET	В	134		88.040	38.474	-5.083	1.00	20.00	6
	ATOM	513	CB	MET	В	134		88.004	37.879	-6.492	1.00	20.00	6
15	ATOM	514	CG	MET	В	134		87.183	36.603	-6.573	1.00	20.00	6
	ATOM	515	SD	MET	В	134		87.477	35.650	-8.077	1.00	20.00	16
	ATOM	516	CE	MET	В	134		88.730	34.515	-7.475	1.00	20.00	6
	ATOM	517	С	MET	В	134		89.115	39.552	-4.994	1.00	20.00	6
	MOTA	518	.0	MET	В	134		90.253	39.264	-4.626	1.00	20.00	8
20	MOTA	519	N	SER	В	135		88.758	40.790	-5.319	1.00	20.00	7
	MOTA	520	CA	SER	В	135		89.708	41.899	-5.260		20.00	6
	MOTA	521	CB	SER	В	135		89.084	43.175	-5.836		20.00	6,
	ATOM	522	OG	SER	В	135		88.742	43.009	-7.202		20.00	8
	MOTA	523	C	SER	В	135		90.165	42.184	-3.830		20.00	6
25	MOTA	524	0	SER				91.228	42.762	-3.614		20.00	8
	MOTA	525	N	ARG				89.354	41.782	-2.857		20.00	7
	MOTA	526	CA	ARG				89.672	42.013	-1.450		20.00	6
	MOTA	527	CB	ARG				88.384	42.156	-0.637		20.00	6
	MOTA	528	CG	ARG				87.509	43.336	-1.018		20.00	6 6
30	ATOM	529	CD	ARG				86.215	43.306	-0.211		20.00	7
	MOTA	530	NE	ARG				86.491	43.117	1.209		20.00	6
	ATOM	531	CZ	ARG				85.565	42.888	2.132 1.786		20.00	7
	ATOM	532		ARG				84.285 85.920	42.821 42.715	3.401		20.00	7
25	MOTA	533	NH2	ARG ARG		136 136		90.506	40.891	-0.839		20.00	6
35	MOTA	534	C	ARG				91.091	41.054	0.231		20.00	
	ATOM	535	0	LEU				90.556	39.752	-1.515		20.00	
	ATOM	536 537	N CA	LEU		137		91.300	38.609	-1.005		20.00	
	MOTA MOTA	538	CB	LEU				90.665	37.307	-1.504		20.00	
40	ATOM	539	CG	LEU				89.172	37.099	-1.213		20.00	
40	ATOM	540		LEU		137		88.748	35.728	-1.734		20.00	
	ATOM	541		LEU		137		88.897	37.205	0.280		20.00	
	ATOM	542	C	LEU		137		92.771	38.648	-1.402	1.00	20.00	6
	ATOM	543	ō	LEU				93.103	38.871	-2.566	1.00	20.00	8
45	ATOM	544	N	ASP				93.645	38.436	-0.424	1.00	20.00	7
	ATOM	545	CA	ASP				95.086	38.422	-0.656	1.00	20.00	6
	MOTA	546	СВ	ASP				95.696	39.797	-0.352	1.00	20.00	6
	ATOM	547	CG	ASP				97.179	39.854	-0.674	1.00	20.00	6
	MOTA	548	OD1	ASP	В	138		97.601	39.173	-1.634		20.00	
50	ATOM .	549	OD2	ASP	В	138		97.920	40.581	0.022		20.00	
	MOTA	550	C	ASP				95.678	37.369	0.263		20.00	
	MOTA	551	0	ASP	В	138		96.353	37.685	1.243		20.00	
	ATOM	552	·N	HIS				95.410	36.111			20.00	
	MOTA	553	CA	HIS				95.871	34.984	0.731		20.00	
55	MOTA	554	CB	HIS				94.769	34.610	1.737		20.00	
	MOTA	555	CG	HIS				95.173	33.561	2.725		20.00	
	MOTA	556	-	HIS				95.543	33.657	4.025		20.00	
	MOTA	557		HIS				95.241	32.221	2.405		20.00	
	MOTA	558	CE1	HIS	В	139		95.635	31.537	3.466	1.00	, 20.00	, 0

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	MOTA	559	NE2	HIS I	В :	139		95.825	32.385	4.461	1.00 20.0	
	ATOM	560	С	HIS 1	в:	139		96.176	33.828	-0.221	1.00 20.0	
	ATOM	561	0	HIS I	в :	139		95.444	33.595	-1.182	1.00 20.0	
	MOTA	562	N	PRO 1	B :	140		97.257	33.080	0.038	1.00 20.0	
5	MOTA	563	CD	PRO 1	в:	140		98.128	33.140	1.225	1.00 20.0	
	MOTA	564	CA	PRO 1	В:	140		97.635	31.959	-0.827	1.00 20.0	
	ATOM	565	CB	PRO 1	В :	140		98.913	31.433	-0.171	1.00 20.0	
	MOTA	566	CG	PRO 1	В :	140		98.687	31.730	1.277	1.00 20.0	
	ATOM	567	С	PRO :	в :	140		96.614	30.846	-1.072	1.00 20.0	
10	ATOM	568	O.	PRO :	В :	140		96.747	30.107	-2.044	1.00 20.0	
•	ATOM	569	N .	PHE :	В :	141		95.607	30.712	-0.211	1.00 20.0	
	ATOM	570	CA	PHE :	В :	141		94.620	29.649	-0.398	1.00 20.0	
	ATOM	571	CB	PHE :	В :	141		94.206	29.056	0.961	1.00 20.0	
	MOTA	572	CG	PHE :	В	141		95.321	28.335	1.681	1.00 20.0	
15	MOTA	573	CD1	PHE	В	141		96.351	27.716	0.967	1.00 20.0	
	ATOM	574	CD2	PHE	В	141		95.311	28.227	3.067	1.00 20.0	
	MOTA	575	CE1	PHE	В	141		97.350	27.000	1.627	1.00 20.0	
,	MOTA	576	CE2	PHE	В	141		96.307	27.510	3.740	1.00 20.0	
	MOTA	577	CZ	PHE	В	141		97.328	26.895	.3.018	1.00 20.0	
20	MOTA	578	С	PHE	В	141		93.371	30.063	-1.181	1.00 20.0	
	ATOM	579	0	PHE	В	141		92.335	29.398	-1.114	1.00 20.0	
	MOTA	580	N	PHE	В	142		93.471	31.150	-1.934	1.00 20.0	
	MOTA	581	CA	PHE	В	142		92.337	31.625	-2.721	1.00 20.0	
	ATOM	582	CB	PHE	В	142		91.739	32.883	-2.082	1.00 20.0	
25	ATOM	583	CG	PHE	В	142		91.048	32.628	-0.772	1.00 20.0	
	MOTA	584	CD1	PHE	В	142		89.715	32.227	-0.740	1.00 20.0	
	ATOM	585	CD2	PHE	В	142		91.741	32.747	0.429	1.00 20.0	
	MOTA	586	CE1	PHE	В	142		89.080	31.944	0.472	1.00 20.0	
	ATOM	587	CE2	PHE	В	142		91.116	32.465	1.647	1.00 20.0	
30	MOTA	588	CZ	PHE	В	142		89.785	32.064	1.667	1.00 20.0	
	MOTA	589	C	PHE	В	142		92.758		-4.146	1.00 20.0	
	MOTA	590	0	PHE	В	142		93.865	32.429	-4.371	1.00 20.0	
	MOTA	591	N	VAL	В	143		91.883	31.653	-5.106	1.00 20.0	
	MOTA	592	CA	VAL	В	143		92.167	31.960	-6.504	1.00 20.0	
35	MOTA	593	CB	VAL				91.009	31.513	-7.435	1.00 20.0	
	MOTA	594	CG1	VAL	В	143	•	91.116	32.209	-8.795	1.00 20.0	
	ATOM	595		VAL				91.061	30.000	-7.623	1.00 20.0	
	ATOM	596	С	VAL				92.301	33.469	-6.545	1.00 20.0	•
	MOTA	597	0	VAL				91.505	34.179	-5.932	1.00 20.0	
40	ATOM	598	N	LYS				93.312	33.957	-7.252	1.00 20.0	
	MOTA	599	CA	LYS				93.547	35.392	-7.340	1.00 20.0	
	ATOM	600	CB	LYS				95.051	35.689	-7.267	1.00 20.0	
	ATOM	601	CG	LYS		144		95.382	37.182	-7.318	1.00 20.0	
	ATOM	602	CD	LYS				96.881	37.441	-7.201	1.00 20.0	
45	ATOM	603	CE	LYS				97.191	38.936	-7.298	1.00 20.0	
	MOTA	604	NZ	LYS				98.661	39.215	-7.246	1.00 20.0	
	ATOM	605	C	LYS				92.989	36.003	-8.614	1.00 20.0	
	MOTA	606	0	LYS				92.993	35.371	-9.675	1.00 20.0	
	ATOM	607	N	LEU				92.495	37.230	-8.490	1.00 20.0	
50	MOTA	608	CA	LEU				91.968	37.975	-9.624 -9.234	1.00 20.0	
	MOTA	609	СВ	LEU				90.678	38.703		1.00 20.	
	ATOM	610	CG	LEU				89.938		-10.326	1.00 20.	
	ATOM	611		LEU				88.611	39.992	-9.782 -10.806	1.00 20.	
	MOTA	612		LEU				90.791 93.059	40.652 38.984	-9.968	1.00 20.	
55	MOTA	613	C	LEU				93.059	39.940	-9.216	1.00 20.	
	MOTA	614	0	LEU				93.735		-11.093	1.00 20.	
	MOTA	615	N			146		94.815		-11.517	1.00 20.	
	ATOM	616	CA			146		95.821		-12.389	1.00 20.	
•	MOTA	617	CB	TAK	Ħ	146		33.04I	30.304	12.309		- •

	MOTA	618	CG	TYR :	В	146	•	96.624	37.858 -11.6	61	1.00	20.00	6
	MOTA	619	CD1	TYR	В	146		96.139	36.559 -11.4	98	1.00	20.00	6
	MOTA	620	CE1	TYR	В	146		96.894	35.589 -10.8	336	1.00	20.00	6
	MOTA	621	CD2	TYR	В	146		97.878	38.165 -11.3	40	1.00	20.00	6
5	ATOM	622	CE2	TYR	В	146		98.639	37.208 -10.4	76	1.00	20.00	6
	ATOM	623	CZ	TYR	В	146		98.144	35.925 -10.3	31	1.00	20.00	6
	ATOM	624	OH	TYR	В	146		98.920	34.981 -9.7	706	1.00	20.00	8
	ATOM	625	C	TYR	В	146		94.357	40.884 -12.2	293	1.00	20.00	6
	ATOM	626	0	TYR	В	146		94.933	41.963 -12.3	60	1.00	20.00	8
10	ATOM	627	N	PHE	B.	147		93.326	40.722 -13.3	110	1.00	20.00	7
	MOTA	628	CA	PHE	В	147		92.855	41.832 -13.9	23	1.00	20.00	6
	MOTA	629	CB	PHE	В	147		93.823	42.044 -15.0	92	1.00	20.00	6
	MOTA	630	CG	PHE	В	147		94.027	40.809 -15.	945	1.00	20.00	6
	ATOM	631	CD1	PHE	В	147		93.049	40.397 -16.8	350	1.00	20.00	6
15	MOTA	632	CD2	PHE	В	147		95.188	40.047 -15.8	322	1.00	20.00	6
	ATOM	633	CE1	PHE	В	147		93.221	39.247 ~17.0			20.00	6
	ATOM	634	CE2	PHE	В	147		95372	38.893 -16.9	585	1.00	20.00	6
	MOTA	635	CZ	PHB	В	147		94.388	38.490 -17.4	185	1.00	20.00	6
	ATOM	636	С	PHE	В	147		91.473	41.566 -14.	180	1.00	20.00	6
20	ATOM	637	0	PHE	В	147		90.972	40.442 -14.	123	1.00	20.00	8
	ATOM	638	N	THR	В	148		90.865	42.616 -15.	021	1.00	20.00	7
	MOTA	639	CA	THR	В	148		89.560	42.509 -15.	543	1.00	20.00	6
	ATOM	640	CB	THR	в	148		88.402	42.889 -14.	578	1.00	20.00	6
	ATOM	641	OG1	THR	В	148	•	88.492	44.275 -14.	338	1.00	20.00	`8
25	ATOM	642	CG2	THR	В	148		88.460	42.057 -13.	403	1.00	20.00	б
	ATOM	643	С	THR	В	148		89.532	43.469 -16.	821	1.00	20.00	6
	ATOM	644	0	THR				90.281	44.448 -16.	866	1.00	20.00	8
•	ATOM	645	N	PHE	В	149		88.685	43.161 -17.	791	1.00	20.00	.7
	ATOM	646	CA	PHE	В	149		88.508	44.011 -18.	948	1.00	20.00	6
30	ATOM	647	CB	PHE	В	149		89.750	44.013 -19.	864		20.00	6
	ATOM	648	CG	PHE	В	149		90.133	42.664 -20.	419	1.00	20.00	6
	ATOM	649	CD1	PHE	В	149		89.552	42.182 -21.	587		20.00	6
	ATOM	650	CD2	PHE	В	149		91.122	41.903 -19.	802	1.00	20.00	6
	ATOM	651	CE1	PHE	В	149		89.953	40.965 -22.			20.00	6
35	ATOM	652	CE2	PHE	В	149		91.532	40.681 -20.	345	1.00	20.00	6
	ATOM	653	CZ	PHE	В	149		90.948	40.213 -21.	517	1.00	20.00	6
	ATOM	654	C	PHE	В	149		87.271	43.498 -19.	649		20.00	6
*	MOTA	655	0	PHE	В	149		86.714	42.474 -19.	251	1.00	20.00	8
	ATOM	656	N	GLN	В	150		86.812	44.221 -20.			20.00	7
40	ATOM	657	CA	GLN	В	150		85.619	43.807 -21.	372	1.00	20.00	6
	ATOM	658	СВ	GLN	В	150		84.358	44.260 -20.	614		20.00	6
	MOTA	659	CG	GLN	В	150		84.302	45.761 -20.			20.00	6
	MOTA	660	CD	GLN	В	150		83.011	46.172 -19.	567		20.00	6
	MOTA	661	OE1	GLN	В	150	•	81.970	46.385 -20.			20.00	8
45	ATOM	662	NE2	GLN	В	150		83.078	46.273 -18.			20.00	7
	ATOM	663	C	GLN	В	150		85.598				20.00	6
	ATOM	664	0	GLN	В	150		86.281	45.387 -23.			20.00	8
	ATOM	665	N	ASP	В	151		84.846	43.766 -23.			20.00	7
	ATOM	666	CA	ASP	В	151		84.683	44.296 -24.			20.00	6
50	MOTA	667	CB	ASP	В	151		85.160	43.312 -26.			20.00	6
	ATOM	668	CG	ASP	В	151		84.558	41.934 -25.			20.00	6
	MOTA	669	OD1	ASP				83.425	41.812 -25.			20.00	8
	MOTA	670		ASP				85.227	40.963 -26.			20.00	8
	MOTA	671	C			151		83.188	44.573 -25.			20.00	6
55	MOTA	672	0			151		82.501	44.610 -24.			20.00	8
	MOTA	673	N	ASP	В	152	•	82.669	44.758 -26.			20.00	7
	MOTA	674	CA			152		81.251	45.062 -26.			2.0.00	6
	MOTA	675	CB			152		80.907	45.346 -27.			20.00	6
	MOTA	676	CG	ASP	В	152		81.616	46.574 -28	432	1.00	20.00	6

	ATOM	677	OD1 A	ASP B	152	81.748		-27.666	1.00 20.00	8
	MOTA	678	OD2 I	ASP B	152	82.030		-29.613	1.00 20.00	8
	MOTA	679	C I	ASP B	152	80.285		-25.888	1.00 20.00	6
	ATOM	680	0 1	ASP B	152	79.229		-25.357	1.00 20.00	8
5	MOTA	681	N (GLU B	153	80.641		-25.982	1.00 20.00	7
	MOTA	682	CA (GLU B	153	79.727		-25.521	1.00 20.00	6
	MOTA	683		GLU B		79.516		-26.641	1.00 20.00	6
	MOTA	684	CG (GLU B	153	79.577		-28.058	1.00 20.00	6
	ATOM	685		GLU B		81.006		-28.550	1.00 20.00	6
10	ATOM	686	OE1	GLU B	153	81.765		-28.635	1.00 20.00	8
	ATOM	687	OE2	GLU B	153	81.374		-28.854	1.00 20.00	8 6
	MOTA	688	C	GLU B	153	80.102		-24.247	1.00 20.00	8
	MOTA	689	0	GLU B	153	79.222		-23.535	1.00 20.00	7
	MOTA	690	N	LYS B	154	81.393		-23.944	1.00 20.00	6
15	ATOM	691	CA	LYS B	154	81.818		-22.787	1.00 20.00	
	MOTA	692		LYS B		82.549		-23.273	1.00 20.00	6
	MOTA	693	CG	LYS B	154	81.785		-24.278	1.00 20.00	6 6
	MOTA	694	CD	LYS B	154	82.727		-25.021	1.00 20.00	6
	MOTA	695		LYS B		81.968		-25.952	1.00 20.00	7
20	MOTA	696	NZ	LYS B	154	82.894		-26.826	1.00 20.00	6
-	MOTA	697	С	LYS B	154	82.709		-21.756	1.00 20.00	8
	MOTA	698	0	LYS B		83.412		-22.048	1.00 20.00	7
	MOTA	699	N	LEU B	155	82.677		-20.551	1.00 20.00	6
	MOTA	700	CA	LEU B	155	83.503		-19.428		6
25	MOTA	701	CB	LEU B	155	82.70			1.00 20.00	6
	MOTA	702	CG		155	81.45		-18.004	1.00 20.00	6
	MOTA	703		LEU B		80.80		-16.645	1.00 20.00	6
	MOTA	704	CD2	LEU B		81.83		-18.152	1.00 20.00	6
	MOTA	705	C	TEA B		84.57	- -	-19.302 -19.495	1.00 20.00	8
30	MOTA	706	0	TEA B		84.28		-19.495	1.00 20.00	7
	MOTA	707	N	TYR B		85.80		-18.809	1.00 20.00	6
	MOTA	708	CA	TYR B		86.89		-19.904	1.00 20.00	6
	MOTA	709	CB	TYR B		87.95		-21.324	1.00 20.00	6
	MOTA	710	CĠ	TYR B		87.45		-21.920	1.00 20.00	6
35	MOTA	711		TYR B		86.68		-23.235	1.00 20.00	
	MOTA	712		TYR B		86.23		-23.233	1.00 20.00	_
	MOTA	713	CD2	TYR B		87.74		-23.387	1.00 20.00	_
	MOTA	714	CE2	TYR B		87.28		-23.958	1.00 20.00	_
	ATOM	715	CZ	TYR B		86.53		-25.246	1.00 20.00	_
40	MOTA	716	OH	TYR B		86.08		-17.447	1.00 20.00	
	MOTA	717	C	TYR B		87.56		-17.110	1.00 20.00	
	ATOM	718	0	TYR B		87.97		-16.667	1.00 20.00	
	MOTA	719	N	PHE B		87.65 88.32		-15.367	1.00 20.00	
	MOTA	720		PHE B	157	•		-14.246	1.00 20.00	
45	ATOM	721		PHE B		87.44 86.19		-13.968	1.00 20.00	
	MOTA	722	CG	PHE B		85.98		-14.535	1.00 20.00	
	ATOM	723	CDI	PHE B	107	85.20		-13.143		
	ATOM	724		PHE B	157	84.80	B 40 324	-14.290		
	MOTA	725		PHE E		84.02		-12.893		
50	MOTA	726				83.82		-13.470		
	ATOM	727		PHE E		89.57		-15.471		_
	ATOM	728		PHE E		89.49	36.10	-15.765	1.00 20.00	
	MOTA	729		GLY E		90.74	12 37.89	3 -15.231		
	ATOM	730		GLY E		91.98	35 37.14	5 -15.303	1.00 20.00) 6
55	ATOM	731		GLY E		92.25	36.51	2 -13.955	1.00 20.0	0 6
	MOTA	732		GLY I		92.5	75 37.21	1 -12.996	1.00 20.0	0 8
	ATOM	733		LEU I	159	92.1		1 -13.886	1.00 20.0	0 7
	ATOM	734		LEU I	3 159	92.3		6 -12.634		
	ATOM	735	5 CA	77770 1		,,,,,				

	ATOM	736	CB	LEU E	3 159	91.116	33.580 -12.358	1.00 20.00	6
	ATOM	737	CG	LEU F	3 159	89.724	34.208 -12.490	1.00 20.00	6
	ATOM	738	CD1	TEA E	3 159	88.670	33.111 -12.398	1.00 20.00	б
	MOTA	739	CD2	LEU E	3 1.59	89.513	35.246 -11.404	1.00 20.00	6
5	MOTA	740	C	LEU E	3 159	93.562	33.582 -12.643	1.00 20.00	6
	MOTA	741	0	LEU E	3 159	94.061	33.204 -13.698	1.00 20.00	8
	ATOM	742	N	SER E	3 160	94.046	33.237 -11.457	1.00 20.00	7
	ATOM	743	CA	SER E	3 160	95.192	32.356 -11.377	1.00 20.00	6
	ATOM	744	CB	SER I	3 160	95.665	32.206 -9.926	1.00 20.00	6
10	ATOM	745	OG	SER F	3 160	94.591	31.973 -9.042	1.00 20.00	8
	ATOM	746	С	SER I	3 160	94.754	31.012 -11.951	1.00 20.00	6
	ATOM	747	0	SER I	3 160	93.598	30.605 -11.813	1.00 20.00	8
	MOTA	748	N	TYR I	3 161	95.674	30.339 ~12.625	1.00 20.00	7
	ATOM	749	CA	TYR I	3 161	95.381	29.050 -13.231	1.00 20.00	6
15	ATOM	750	CB	TYR I	3 161	96.170	28.924 -14.543	1.00 20.00	6
	ATOM	751	CG	TYR I	3 161	96.128	27.564 -15.209	1.00 20.00	6
	ATOM	752	CD1	TYR I	B 161	94.968	26.787 -15.193	1.00 20.00	6
	ATOM	753	CEl	TYR I	B 161	94.915	25.554 -15.846	1.00 20.00	6
	ATOM	754	CD2	TYR I	B 161	97.240	27.073 -15.895	1.00 20.00	6
20	ATOM	755	CE2	TYR	B 161	97.198	25.841 -16.553	1.00 20.00	6
	MOTA	756	CZ	TYR I	B 161	96.033	25.088 -16.523	1.00 20.00	6
	ATOM	757	OH	TYR 1	B 161	95.983	23.877 -17.173	1.00 20.00	8
	ATOM	758	С	TYR I	B 161	95.724	27.905 -12.277	1.00 20.00	6
	MOTA	759	0	TYR !	B 161	96.897	27.598 -12.065	1.00 20.00	8
25	MOTA	760	N	ALA :	B 162	94.696	27.288 -11.697	1.00 20.00	.7
	MOTA	761	CA	ALA :	B 162	94.893	26.166 -10.776	1.00 20.00	6
	MOTA	762	CB	ALA :	B 162	93.666	25.995 -9.873	1.00 20.00	6
	ATOM	763	C	ALA :	B · 162	95.100	24.924 -11.637	1.00 20.00	6
	MOTA	764	0	ALA	B 162	94.146	24.251 -12.015	1.00 20.00	8
30	ATOM	765	N		в 163	96.361	24.626 -11.930	1.00 20.00	7
	ATOM	766	CA		в 163	96.722	23.506 -12.795	1.00 20.00	6
	ATOM	767	CB		B 163	98.247	23.416 -12.912	1.00 20.00	6
	ATOM	768	CG		в 163	98.904	24.711 -13.360	1.00 20.00	6
	MOTA	769	CD		B 163	100.405	24.539 -13.554	1.00 20.00	6 6
35	MOTA	770	CE		B 163	101.102	25.885 -13.690		7
	MOTA	771	NZ		B.163	100.976	26.701 -12.445		6
	ATOM	772	C		B 163	96.170	22.123 -12.464		8
	ATOM	773	0		B 163	95.823	21.370 -13.369 21.775 -11.186		7
	MOTA	774	N		B 164	96.076	20.449 -10.842		6
40	ATOM	775	CA		B 164	95.594	19.944 -9.610		6
	ATOM	776	CB		B 164	96.339 97.766	19.529 -9.943		6
	ATOM	777	CG		B 164 B 164	97.700	18.776 -10.892		8
	MOTA	778			B 164	98.730	20.014 -9.171		7
4.5	ATOM	779			B 164	94.084	20.246 -10.706		6
45	ATOM	780	C		B 164	93.630	19.183 -10.286		8
	ATOM	781	0		B 165	93.309	21.257 -11.080		7
	ATOM	782	N CA		B 165	91.863	21.127 -11.039		6
	MOTA	783	C		B 165	91.159	21.088 -9.694		6
50	MOTA	784 785	0		B 165	91.663	21.598 -8.698		8
50	ATOM ATOM	786	N		B 166	89.986	20.461 -9.689		7
	MOTA	787	CA		B 166	89.126	20.344 -8.513		6
	ATOM	788	CB		B 166	87.683	20.079 -8.962		6
	ATOM	789	CG		B 166	86.992	21.255 -9.646		6
55	ATOM	790	CD		B 166	85.709	20.837 -10.358	1.00 20.00	6
55	ATOM	791	OE1		B 166	85.137	19.794 -9.986	1.00 20.00	8
	ATOM	792	OE2		B 166		21.556 -11.279	1.00 20.00	8
	ATOM	793	C		B 166		19.270 -7.506	1.00 20.00	6
	ATOM	794	ō		B 166		18.184 -7.874	1.00 20.00	8

	MOTA	795	N	LEU	В	167	89.344	19.579	-6.226	1.00 20.00	7
	MOTA	796	CA	LEU	В	167	89.651	18.626	-5.168	1.00 20.00	6
	ATOM	797	CB	LEU	В	167	89.395	19.269	-3.802	1.00 20.00	6
	MOTA	798	CG	LEU	В	167	89.408	18.363	-2.569	1.00 20.00	6
5	ATOM	799	CD1	LEU	В	167	90.769	17.703	-2.412	1.00 20.00	6
_	ATOM	800		LEU		167	89.065	19.193	-1.338	1.00 20.00	6
	ATOM	801	C	LEU		167	88.757	17.394	-5.346	1.00 20.00	6
	ATOM	802	ō	LEU			89.124	16.283	-4.968	1.00 20.00	8
				LEU		168	87.580	17.600	-5.927	1.00 20.00	7
10	MOTA	803	N					16.500	-6.153	1.00 20.00	6
10	MOTA	804	CA	LEU		168	86.647				6
	MOTA	805	CB	LEU		168	85.364	17.014	-6.809	1.00 20.00	
	ATOM	806	CG	LEU		168	84.292	15.977	-7.168	1.00 20.00	6
	ATOM	807	CD1	LEU	В	168	83.883	15.186	-5.929	1.00 20.00	6
	MOTA	808	CD2	LEU	В	168	83.083	16.687	-7.756	1.00 20.00	6
15	MOTA	809	С	LEU	В	168	87.290	15.440	-7.046	1.00 20.00	6
	MOTA	810	0	LEU	В	168	87.091	14.243	-6.845	1.00 20.00	8
	ATOM	811	N	LYS	В	169	88.068	15.888	-8.027	1.00 20.00	7
	ATOM	812	CA	LYS	в	169	88.727	14.967	-8.941	1.00 20.00	6
	ATOM	813	CB	LYS		169	89.610	15.729	-9.930	1.00 20.00	6
20	ATOM	814	CG	LYS		169	90.379		-10.882	1.00 20.00	б
20		815	CD	LYS		169	91.226		-11.877	1.00 20.00	6
	MOTA			LYS		169	92.373		-11.192	1.00 20.00	6
	MOTA	816	CE				93.253		-12.173	1.00 20.00	7
	MOTA	817	NZ	LYS		169		13.949	-8.193	1.00 20.00	6
	MOTA	818	С	LYS		169	89.574			1.00 20.00	8
25	MOTA	819	0	LYS		169	89.543	12.758	-8.504		7
	MOTA	820	N	TYR		170	90.334	14.417	-7.207	1.00 20.00	6
	MOTA	821	CA	TYR		170	91.197	13.527	-6.441	1.00 20.00	
	MOTA	822	CB	TYR		170	92.243	14.346	-5.682	1.00 20.00	6
	MOTA	823	CG	TYR		170	93.217	15.010	-6.624	1.00 20.00	6,
30	MOTA	824	CD1	TYR			94.347	14.331	-7.085	1.00 20.00	6
	MOTA	825	CE1	TYR	В	170	95.195	14.900	-8.036	1.00 20.00	6
	MOTA	826	CD2	TYR	В	170	92.963	16.282	-7.133	1.00 20.00	6
	MOTA	827	CE2	TYR	В	170	93.801	16.861	-8.083	1.00 20.00	6
	ATOM	828	\mathbf{cz}	TYR	В	170	94.913	16.164	-8.532	1.00 20.00	6
35	ATOM	829	OH	TYR	В	170	95.727	16.727	-9.493	1.00 20.00	8
	ATOM	830	C	TYR	В	170	90.419	12.622	-5.499	1.00 20.00	6
	ATOM	831	O	TYR	В	170	90.834	11.494	-5.233	1.00 20.00	8
	ATOM	832	N	ILE			89.287	13.098	-4.993	1.00 20.00	7
	ATOM	833	CA	ILE			88.488	12.262	-4.112	1.00 20.00	6
40	MOTA	834	СВ	ILE			87.278	13.028	-3.538	1.00 20.00	6
40	ATOM	835	CG2	ILE			86.367	12.065	-2.791	1.00 20.00	6
		836		ILE			87.764	14.141	-2.603	1.00 20.00	6
	ATOM		CD1			171	86.652	14.990	-2.019	1.00 20.00	6
	ATOM	837	C.	ILE			87.994	11.066	-4.931	1.00 20.00	6
	ATOM	838	_						-4.468	1.00 20.00	8
45	ATOM		, 0	ILE						1.00 20.00	7
	MOTA	840	N	ARG			87.550	11.331	-6.156		6
	ATOM	841	CA	ARG			87.061	10.273	-7.031	1.00 20.00	
	ATOM	842	CB			172	86.359	10.861	-8.259	1.00 20.00	6
	ATOM	843	CG	ARG			85.094	11.658	-7.963	1.00 20.00	6
50	MOTA	844	CD	ARG	В	172	84.352	11.981	-9.259	1.00 20.00	6
	ATOM	845	NE	ARG	В	172	83.187	12.843	-9.063	1.00 20.00	7
	ATOM	. 846	CZ	ARG	В	172	82.192	12.589	-8.217	1.00 20.00	6
	MOTA	847	NH1	ARG	В	172	82.209	11.491	-7.469	1.00 20.00	
	ATOM	848	NH2	ARG	В	172	81.168	13.428	-8.127	1.00 20.00	
55	ATOM	849	С	ARG	В	172	88.202	9.378	-7.497	1.00 20.00	
	ATOM	850	0	ARG	В	172	88.050	8.160	-7.587	1.00 20.00	
	ATOM	851	N			173	89.348	9.985	-7.783	1.00 20.00	7
	ATOM	852	CA			173	90.509	9.244	-8.256	1.00 20.00	6
	MOTA	853	СВ			173	91.647	10.206	-8.603	1.00 20.00	6
	A1014	0.00	2,5		_		52.01.				

	MOTA	854	CG	LYS I	В	173		92.930	9.511	-9.045	1.00 20.00	6
	ATOM	855	CD	LYS :	В	173		94.081	10.496	-9.222	1.00 20.00	6
	MOTA	856	CE	LYS :	В	173		93.862	11.432	-10.406	1.00 20.00	6
	MOTA	857	NZ	LYS :	В	173		93.858	10.711	~11.715	1.00 20.00	7
5	ATOM	858	C	LYS :	В	173		91.025	8.191	-7.280	1.00 20.00	6
	ATOM	859	0	LYS :		173		91.274	7.055	-7.674	1.00 20.00	8
	ATOM	860	N	ILE	В	174		91.192	8.554	-6.012	1.00 20.00	7
	MOTA	861	CA	ILE	В	174		91.710	7.593	-5.042	1.00 20.00	6
	MOTA	862	CB	ILE :	В	174		92.884	8.191	-4.223	1.00 20.00	6
10	ATOM	863	CG2	ILE	В	174		93.970	8.701	-5.166	1.00 20.00	6
	ATOM	864	CG1	ILE	В	174		92.394	9.337	-3.343	1.00 20.00	6
	ATOM	865	CD1	ILE	В	174		93.480	9.916	-2.457	1.00 20.00	6
	MOTA	866	C	ILE	В	174		90.674	7.030	-4.074	1.00 20.00	6
	ATOM	867	0	ILE	В	174		91.025	6.296	-3.151	1.00 20.00	8
15	ATOM	868	N	GLY	В	175		89.405	7.367	-4.283	1.00 20.00	7
	MOTA	869	CA	GLY	В	175		88.359	6.855	-3.413	1.00 20.00	6
	ATOM	870	С	GLY	В	175		88.160	7.650	-2.138	1.00 20.00	6
	MOTA	871	0	GLY	В	175		87.083	8.198	-1.905	1.00 20.00	8
	MOTA	872	N	SER	В	176		89.192	7.701	-1.304	1.00 20.00	7
20	ATOM	873	CA	SER	В	176		89.140	8.447	-0.053	1.00 20.00	6
	ATOM	874	CB	SER '	В	176		88.395	7.653	1.026	1.00 20.00	6
	ATOM	875	OG	SER	В	176		89.150	6.543	1.472	1.00 20.00	8
	MOTA	876	С	SER	В	176		90.565	8.742	0.401	1.00 20.00	6
	MOTA	877	0	SER	В	176		91.506	8.049	0.009	1.00 20.00	8
25	ATOM	878	N	PHE	В	177		90.718	9.769	1.228	1.00 20.00	7
	MOTA	879	CA ·	PHE	В	177		92.029	10.184	1.722	1.00 20.00	6
	MOTA	880	CB	PHE	В	177		92.028	11.694	1.990	1.00 20.00	6
	ATOM	881	CG	PHE	B	177		92.002	12.546	0.747	1.00 20.00	6
	ATOM	882	CD1	PHE	В	177		91.484	12.060	-0.449	1.00 20.00	6
30	ATOM	883	CD2	PHE	В	177		92.481	13.855	0.787	1.00 20.00	6
	ATOM	884	CE1	PHE	В	177		91.443	12.860	-1.585	1.00 20.00	é
	ATOM	885	CE2	PHE	В	177		92.444	14.665	-0.343	1.00 20.00	6
	ATOM	886	CZ	PHE	В	177		91.925	14.168	-1.532	1.00 20.00	6
	ATOM	887	C	PHE	В	177		92.427	9.475	3.009	1.00 20.00	6
35	MOTA	888	o í	PHE	В	177		91.582	9.223	3.872	1.00 20.00	8
	ATOM	889	N	ASP	В	178		93.711	9.152	3.147	1.00 20.00	7
	MOTA	890	CA	ASP	В	178		94.155	8.529	4.385	1.00 20.00	6
	ATOM	891	CB	ASP	В	178		95.581	7.972	4.267	1.00 20.00	6
	MOTA	892	CG	ASP	В	178		96.594	9.018	3.845	1.00 20.00	6
40	ATOM	893	OD1	ASP	В	178		96.392	10.214	4.139	1.00 20.00	8
	ATOM	894	QD2	ASP	В	178		97.612	8.634	3.230	1.00 20.00	8
	ATOM	895	С	ASP	В	178		94.092	9.640	5.436	1.00 20.00	6
	ATOM	896	Ö	ASP	В	178		93.736	io.778	5.117	1.00 20.00	8
	ATOM	897	N	GLU	В	179		94.443	9.324	6.677	1.00 20.00	7
45	ATOM	898	CA	GLU	В	179		94.380	10.311	7.744	1.00 20.00	6
	ATOM	899	CB	GLU	B	179		94.623	9.637	9.096	1:00 20.00	6
	ATOM	900	CG	GLU	В	179		94.747	10.611	10.255	1.00 20.00	6
	ATOM	901	CD	GLU	В	179		94.331	9.994	11.574	1.00 20.00	6
	ATOM	902	OE1	GLU	В	179		94.589	8.789	11.770	1.00 20.00	8
50	ATOM	903	OE2	GLU	В	179		93.753	10.717	12.416	1.00 20.00	8
50	ATOM	904	C ·	GLU	В	179		95.320	11.501	7.575	1.00 20.00	6
	ATOM	905	0			179		94.948	12.636	7.881	1.00 20.00	8
	ATOM	906	N			180		96.528	11.246	7.086	1.00 20.00	7
	MOTA	907	CA			180		97.509	12.308	6.886	1.00 20.00	6
55	MOTA	908	CB			180		98.866	11.720	6.445	1.00 20.00	6
	ATOM	909	OG1	THR				99.349	10.842	7.466	1.00 20.00	
	ATOM	910	CG2			180		99.888	12.825	6.213	1.00 20.00	
	ATOM	911	C			180		97.040	13.331	5.849	1.00 20.00	
	ATOM	912	0			180	•	97.136	14.542		1.00 20.00	8

	ATOM	913	N	CYS	В	181	96.534	12.845	4.721	1.00 20.00	7
	ATOM	914	CA	CYS	В	181	96.057	13.733	3.666	1.00 20.00	6
	ATOM	915	CB	CYS	В	181	95.836	12.945	2.375	1.00 20.00	6
	MOTA	916	SG	CYS	В	181	97.372	12.255	1.685	1.00 20.00 1	.6
5	ATOM	917	C	CYS	В	181	94.775	14.449	4.079	1.00 20.00	6
	ATOM	918	0	CYS	В	181	94.570	15.615	3.733	1.00 20.00	8
	MOTA	919	N	THR	В	182	93.914	13.755	4.820	1.00 20.00	7
	MOTA	920	CA	THR	В	182	92.669	14.356	5.286	1.00 20.00	6
	MOTA	921	CB	THR	В	182	91.812	13.354	6.103	1.00 20.00	6
10	ATOM	922	OG1	THR	В	182	91.372	12.283	5.259	1.00 20.00	8
	ATOM	923	CG2	THR	В	182	90.600	14.054	6.690	1.00 20.00	6
	ATOM	924	С	THR	В	182	93.014	15.535	6.196	1.00 20.00	6
	ATOM	925	0	THR	В	182	92.515	16.649	6.019	1.00 20.00	8
	ATOM	926	N	ARG	В	183	93.873	15.273	7.175	1.00 20.00	7
15	ATOM	927	CA	ARG	В	183	94.299	16.293	8.121	1.00 20.00	6
	ATOM	928	CB	ARG	В	183	95.311	15.707	9.109	1.00 20.00	6
	ATOM	929	CG	ARG		183	95.957	16.744	10.012	1.00 20.00	6
	ATOM	930	CD	ARG	В	183	96.886	16.116	11.050	1,00 20.00	6
	MOTA	931	NE	ARG	В	183	96.167	15.220	11.949	1.00 20.00	7
20	MOTA	932	CZ	ARG	В	183	96.098	13.900	11.804	1.00 20.00	6
	ATOM	933	NH1	ARG	В	183	96.717	13.306	10.791	1.00 20.00	7
	ATOM	934	NH2	ARG	В	183	95.389	13.176	12.664	1.00 20.00	7
	MOTA	935	C	ARG	В	183	94.923	17.505	7.427	1.00 20.00	6
	MOTA	936	0	ARG	В	183	94.545	18.646	7.698	1.00 20.00	8
25	MOTA	937	N	PHE	В	184	95.877	17.264	6.534	1.00 20.00	7
	MOTA	938	CA	PHE	В	184	96.539	18.367	5.847	1.00 20.00	6
	MOTA	939	CB	PHE			97.610	17.847	4.889	1.00 20.00	6
	MOTA	940	CG	PHE			98.387	18.943	4.223	1.00 20.00	6 6
	ATOM	941		PHE		184	99.451	19.555	4.879	1.00 20.00	6
30	ATOM	942		PHE			98.009	19.415 20.627	2.975 4.301	1.00 20.00	6
	ATOM	943		PHE			100.125 98.676	20.627	2.388	1.00 20.00	6
	ATOM	944		PHE		184	99.735	21.097	3.053	1.00 20.00	6
	ATOM	945	CZ	PHE			95.580	19.267	5.066	1.00 20.00	6
25	ATOM	946	С 0	PHE			95.567	20.481	5.255	1.00 20.00	8
35	ATOM	947	N	TYR			94.784	18.679	4.181	1.00 20.00	7
	ATOM	948 949	CA	TYR		185	93.854	19.471	3.390	1.00 20.00	6
	ATOM	950	CB			185	93.305	18.634	2.236	1.00 20.00	6
	ATOM ATOM	951	CG			185	94.337	18.504	1.140	1.00 20.00	6
40	ATOM	952		TYR			94.611	19.580	0.293	1.00 20.00	6
70	ATOM	953	CE1			185	95.637	19.516	-0.643	1.00 20.00	6
	ATOM	954	CD2				95.118	17.352	1.017	1.00 20.00	6
	ATOM	955	CE2			185	96.152	17.282	0.081	1.00 20.00	6
	ATOM	956	CZ			185	96.405	18.367	-0.742	1.00 20.00	6
45	ATOM	957	ОН	TYR	В	185	97.436	18.314	-1.657	1.00 20.00	8
	ATOM	958	C			185	92.738	20.098	4.208	1.00 20.00	6
	ATOM	959	0	TYR	В	185	92.286	21.195	3.891	1.00 20.00	8
	ATOM	960	N	THR	В	186	92.303	19.422	5.267	1.00 20.00	7
	ATOM	961	CA	THR	В	186	91.265	19.987	6.122	1.00 20.00	6
50	ATOM	962	CB	THR	В	186		18.996	7.219	1.00 20.00	6
	MOTA	963	OG1	THR	B	186	-90.193	17.846	6.606	1.00 20.00	8
	MOTA	964	CG2	THR	В	186		19.671	8.144	1.00 20.00	6
	MOTA	965	С			186		21.218	6.805	1.00 20.00	6
	MOTA	966	0			186		22.242	6.948	1.00 20.00	8
55	MOTA	967	N			187		21.115	7.222	1.00 20.00 1.00 20.00	7 6
	ATOM	968	CA			187		22.234	7.882	1.00 20.00	6
	MOTA	969	CB			187		21.817	8.349	1.00 20.00	6
	MOTA	970	C			187		23.449	6.946 7.372	1.00 20.00	8
	MOTA	971	0	ΑĹΆ	В	187	93.654	24.585	1.312	1.00 20.00	3

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GLU B 188 94.205 23.222 5.674 1.00 20.00 MOTA 972 N **GLU B 188** 94.292 24.343 4.740 1.00 20.00 CA ATOM 973 1.00 20.00 6 CB **GLU B 188** 94.843 23.898 3.376 974 ATOM ATOM 975 CG **GLU B 188** 96.285 23.391 3.407 1.00 20.00 6 1.00 20.00 6 CD **GLU B 188** 97.030 23.639 2,104 ATOM 976 1.024 1.00 20.00 96.407 23.537 **GLU B 188** ATOM 977 OE1 1.00 20.00 OE2 GLU B 188 98.247 23.932 2.156 ATOM 978 24.977 4.561 1.00 20.00 6 **GLU B 188** 92.912 MOTA 979 C 1.00 20.00 Я **GLU B 188** 92.782 26.196 4.533 MOTA 980 0 7 ILE B 189 91.875 24.152 4.451 1.00 20.00 MOTA 981 N 4.284 1.00 20.00 6 90.530 24.693 MOTA 982 CA ILE B 189 6 89.495 23.566 4.064 1.00 20.00 ILE B 189 CB ATOM 983 CG2 ILE B 189 88.094 24.157 3.947 1.00 20.00 6 984 ATOM 1.00 20.00 6 89.855 22.773 2.796 MOTA 985 CG1 ILE B 189 1.00 20.00 6 21.488 2.616 .15 ILE B 189 89.058 ATOM 986 CD1 90.152 25.517 5.519 1.00 20.00 987 C **ILE B 189** ATOM 1.00 20.00 8 ILE B 189 89.634 26.630 5.396 MOTA 988 0 7 24.971 6.707 1.00 20.00 VAL B 190 90.412 ATOM 989 N 1.00 20.00 6 90.116 25.674 7.957 990 CA VAL B 190 ATOM 1.00 20.00 б 24.842 9.186 90.557 MOTA 991 CB VAL B 190 90.540 25.717 10.451 1.00 20.00 6 992 CG1 VAL B 190 MOTA 1.00 20.00 89,643 23.641 9.358 6 CG2 VAL B 190 ATOM 993 27.012 7.984 1.00 20.00 6 994 С VAL B 190 90.865 ATOM 8 1.00 20.00 VAL B 190 90.311 28.039 8.375 995 0 ATOM 1.00 20.00 7 92.125 26.997 7.557 N **SER B 191** 25 MOTA 996 7.546 1.00 20.00 6 92.934 28.218 997 CA **SER B 191** MOTA 7.166 1.00 20.00 6 **SER B 191** 94.378 27.888 ATOM 998 CB 1.00 20.00 8 95.220 29.007 7.363 999 OG**SER B 191** MOTA 1.00 20.00 6 6.566 29.240 1000 C **SER B 191** 92.361 MOTA 30.444 6.838 1.00 20.00 8 92.351 30 1001 0 SER B 191 MOTA 5.425 1.00 20.00 7 91.882 28.754 ALA B 192 ATOM 1002 N 4.417 1.00 20.00 ALA B 192 91.306 29.634 6 1003 CA ATOM 1.00 20.00 6 3.141 CB ALA B 192 91.006 28.850 MOTA 1004 4.970 1.00 20.00 90.029 30.256 ALA B 192 MOTA 1005 C 1.00 20.00 8 89.799 31.458 4.822 35 1006 0 ALA B 192 MOTA 5.621 1.00 20.00 7 89.203 29.439 **LEU B 193** MOTA 1007 N 1.00 20.00 6 LEU B 193 87.957 29.941 6.192 1008 CA ATOM 1.00 20.00 6 6.725 87.101 28.783 MOTA 1009 CB LEU B 193 5.650 1.00 20.00 6 86.447 27.898 MOTA 1010 CG LEU B 193 1.00 20.00 6 CD1 LEU B 193 85.645 26.771 6.315 40 MOTA 1011 6 28.752 4.780 1.00 20.00 85.530 1012 CD2 LEU B 193 MOTA 1.00 20.00 7.299 6 88.215 30.959 MOTA 1013 C **LEU B 193** 1.00 20.00 8 LEU B 193 87.474 31.935 7.435 MOTA 1014 O 1.00 20.00 7 89.254 8.100 30.738 ATOM 1015 N **GLU B 194** 9.157 1.00 20.00 6 89.562 31.699 45 MOTA 1016 CA **GLU B 194** 6 1.00 20.00 **GLU B 194** 90.773 31:257 9.982 1017 CB MOTA 1.00 20.00 6 10.914 91.288 32.353 1018 CG **GLU B 194** MOTA 11.855 1.00 20.00 6 92.381 31.878 **GLU B 194** 1019 CD ATOM 8 93.246 31.090 11.420 1.00 20.00 1020 OE1 GLU B 194 ATOM 13.031 8 1.00 20.00 92.376 32.312 50 ATOM 1021 OE2 GLU B 194 1.00 20.00 6 89.847 33.053 8.511 ATOM 1022 **GLU B 194** C 1.00 20.00 8 89.375 8.972 1023 GLU B 194 34.083 MOTA O 1.00 20.00 90.608 7.426 7 33.046 MOTA 1024 N TYR B 195 6 90.928 6.743 1.00 20.00 **TYR B 195** 34.294 1025 CA MOTA 1.00 20.00 б 5.613 1026 CB TYR B 195 91.919 34.043 55 MOTA 1.00 20.00 6 92.193 4.774 35.271 ATOM 1027 CG **TYR B 195** 6 93.098 36.244 5.202 1.00 20.00 1028 CD1 TYR B 195 MOTA 93.356 1.00 20.00 6 37.382 4.429 CE1 TYR B 195 ATOM 1029 1.00 20.00 6 CD2 TYR B 195 91.545 35.461 3.553 1030 MOTA

	ATOM	1031	CE2	TYR	В	195	91.794	36.591	2.775	1.00 20.00	6
	ATOM	1032	CZ	TYR			92.701	37.545	3.219	1.00 20.00	6
	MOTA	1033	OH	TYR			92.956	38.656	2.450	1.00 20.00	В
	ATOM	1034	C	TYR			89.668	34.923	6.160	1.00 20.00	6
5	MOTA	1035	o	TYR			89.409	36.117	6.328	1.00 20.00	8
,								34.103	5.472		
	ATOM	1036	N	LEU			88.885			1.00 20.00	7
	ATOM	1037	CA	LEU			87.664	34.576	4.845	1.00 20.00	6
	ATOM	1038	CB	LEU			86.972	33.426	4.107	1.00 20.00	6
	ATOM	1039	CG	LEU			85.933	33.824	3.060	1.00 20.00	6
10	MOTA	1040		LEU			86.602	34.659	1.966	1.00 20.00	6
	MOTA	1041	CD2	LEU	В	196	85.305	32.568	2.463	1.00 20.00	6
	MOTA	1042	С	LEU	В	196	86.731	35.161	5.888	1.00 20.00	6
	MOTA	1043	0	LEU	В	196	86.299	36.308	5.774	1.00 20.00	8
	ATOM	1044	N	HIS	В	197	86.431	34.378	6.917	1.00 20.00	7
15	MOTA	1045	CA	HIS	В	197	85.533	34.840	7.967	1.00 20.00	6
	ATOM	1046	CB	HIS	В	197	85.241	33.697	8.942	1.00 20.00	6
	ATOM	1047	CG	HIS			84.377	32.622	8.356	1.00 20.00	6
	ATOM	1048		HIS			83.734	32.550	7.163	1.00 20.00	6
	ATOM	1049		HIS			84.083	31.452	9.022	1.00 20.00	7
20	MOTA	1050		HIS			83.296	30.704	8.264	1.00 20.00	6
20		1050		HIS				31.346		1.00 20.00	7
	ATOM						83.071		7.132		
	ATOM	1052	C	HIS			86.080	36.060	8.697	1.00 20.00	6
	ATOM	1053	0	HIS			85.314	36.919	9.146	1.00 20.00	8
	ATOM	1054	Ŋ	GLY			87.404	36.143	8.804	1.00 20.00	7
25	MOTA	1055	CA	GLY			88.009	37.285	9.464	1.00 20.00	6
	MOTA	1056	С	GLY	В	198	87.687	38.580	8.737	1.00 20.00	6
	MOTA	1057	0	GLY	В	198	87.784	39.661	9.311	1.00.20.00	8
	ATOM	1058	N	LYS	В	199	87.308	38.475	7.466	1.00 20.00	7
	MOTA	1059	CA	LYS	В	199	86.959	39.652	6.674	1.00 20.00	6
30	MOTA	1060	CB	ĿYS	В	199	87.577	39.573	5.279	1.00 20.00	6
	ATOM	1061	CG	LYS	В	199	89.082	39.736	5.258	1.00 20.00	6
	ATOM	1062	CD	LYS			89.574	39.919	3.833	1.00 20.00	6
	ATOM	1063	CE	LYS			91.054	40.243	3.807	1.00 20.00	6
	ATOM	1064	NZ	LYS			91.398	41.382	4.706	1.00 20.00	7
35	ATOM	1065		LYS			85.451	39.804	6.539	1.00 20.00	6
55	ATOM	1066	Ö	LYS			84.972	40.556	5.693	1.00 20.00	8
										1.00 20.00	7
	ATOM	1067	N	GLY			84.707	39.079	7.368		
	ATOM	1068	CA	GLY			83.258	39.158	7.328	1.00 20.00	6
4.0	ATOM	1069	C	GLY			82.646	38.660	6.032	1.00 20.00	6
40	MOTA	1070	0	GLY			81.644	39.198	5.564	1.00 20.00	8
	MOTA	1071	N	ILE			83.243	37.630	5.445	1.00 20.00	7
	MOTA	1072	CA	ILE			82.726	37.075	4.205	1.00 20.00	6
	ATOM	1073	CB	ILE	В	201	83.775	37.140	3.080	1.00 20.00	6
	ATOM	1074	CG2	ILE	В	201	83.257	36.413.	1.841	1.00 20.00	6
45	ATOM	1075	CG1	ILE	В	201	84.109	38.599	2.761	1.00 20.00	6
	ATOM	1076	CD1	ILE	В	201	85.330	38.758	1.870	1.00 20.00	6
	ATOM	1077	C	ILE			82.329	35.623	4.395	1.00 20.00	6
	ATOM	1078	0	ILE			83.094	34.826	4.942	1.00 20.00	8
	ATOM	1079	N	ILE			81.125	35.291	3.940	1.00 20.00	7
50	ATOM	1080	CA	ILE			80.592		4.016	1.00 20.00	6
50	ATOM	1081	CB	ILE			79.119	33.953	4.481	1.00 20.00	6
	ATOM	1082		ILE			78.583	32.522	4.595	1.00 20.00	6
				ILE			79.008	34.675	5.825	1.00 20.00	6
	ATOM	1083									
	ATOM	1084		ILE			77.576	34.865	6.294	1.00 20.00	6
55	ATOM	1085	C	ILE			80.644	33.393	2.589	1.00 20.00	6
	MOTA	1086	0	ILE			80.182	34.056	1.663	1.00 20.00	8
	ATOM.	1087	N	HIS			81.204	32.204	2.395	1.00 20.00	7
	MOTA	1088	CA	HIS			81.279	31.652	1.044	1.00 20.00	6
	MOTA	1089	CB	HIS	В	203	82.258	30.480	0.999	1.00 20.00	6

	MOTA	1090	CG	HIS	В	203	82.478	29.942	-0.380	1.00 20.00	6
	ATOM	1091	CD2	HIS	В	203	81.646	29.282	-1.220	1.00 20.00	6
	MOTA	1092	ND1	HIS	В	203	83.659	30.116	-1.069	1.00 20.00	7
	ATOM	1093	CE1	HIS	В	203	83.545	29.588	-2.275	1.00 20.00	6
5	ATOM	1094	NE2	HIS	В	203	82.333	29.076	-2.392	1.00 20.00	7
	ATOM	1095	C	HIS	В	203	79.896	31.211	0.530	1.00 20.00	6
	ATOM	1096	0	HIS			79.508	31.546	-0.593	1.00 20.00	8
	ATOM	1097	N	ARG			79.168	30.458	1.357	1.00 20.00	7
	ATOM	1098	CA	ARG			77.819	29.969	1.039	1.00 20.00	6
10	ATOM	1099	CB	ARG			76.916	31.117	0.583	1.00 20.00	6
10	ATOM	1100	CG	ARG			76.601	32.120	1.675	1.00 20.00	6
	ATOM	1101	CD	ARG			75.316	32.878	1.377	1.00 20.00	6
	ATOM	1102	NE	ARG			75.376	33.616	0.119	1.00 20.00	7
		1102	CZ	ARG			74.423	34.443	-0.303	1.00 20.00	6
15	MOTA	1103		ARG			73.336	34.636	0.436	1.00 20.00	7
15	ATOM							35.084	-1.457	1.00 20.00	7
	ATOM	1105		ARG			74.555		0.030	1.00 20.00	6
	MOTA	1106	C	ARG			77.700	28.829		1.00 20.00	8
	MOTA	1107	0	ARG			76.611	28.300	-0.177		7
	MOTA	1108	N	ASP			78.792	28.456	-0.620	1.00 20.00	6
20	MOTA	1109	CA	ASP			78718	27.342	-1.550	1.00 20.00	
	MOTA	1110	CB	ASP			78.380	27.829	-2.961	1.00 20.00	6
	MOTA	1111	CG	ASP			77.941	26.694	-3.867	1.00 20.00	6
	MOTA	1112		ASP			77.544	25.638	-3.330	1.00 20.00	8
_	MOTA	1113		ASP			77.982	26.853	-5.104	1.00 20.00	8
25	MOTA	1114	C	ASP			80.019	26.560	-1.547	1.00 20.00	6
	MOTA	1115	0	ASP			80.508	26.122	-2.588	1.00 20.00	8
	MOTA	1116	N	TEA.	В	206	80.573	26.375	-0.354	1.00 20.00	7
	MOTA	1117	CA	LEU			81.819	25.652	-0.208	1.00 20.00	6
	MOTA	1118	CB	LEU	B	206	82.361	25.826	1.212	1.00 20.00	6
30	MOTA	1119	CG	LEU	В	206	83.764	25.271	1.471	1.00 20.00	6
	ATOM.	1120	CD1	\mathbf{LEU}	В	206	84.765	25.969	0.561	1.00 20.00	6
	MOTA	1121	CD2	$_{ m LEU}$	В	206	84.135	25.477	2.933	1.00 20.00	6
	ATOM	1122	C	LEU	В	206	81.609	24.174	-0.514	1.00 20.00	6
	MOTA	1123	0			206	80.691	23.549	0.011	1.00 20.00	8
35	ATOM	1124	N	LYS	В	207	82.461	23.628	-1.375	1.00 20.00	7
	ATOM	1125	CA	LYS	В	207	82.379	22.223	-1.765	1.00 20.00	6
	ATOM	1126	CB	LYS	В	207	81.160	22.000	-2.679	1.00 20.00	6
	ATOM	1127	CG	LYS	В	207	81.130	22.913	-3.893	1.00 20.00	6
	ATOM	1128	CD	LYS	В	207	79.876	22.720	-4.736	1.00 20.00	6
40	MOTA	1129	CE	LYS	В	207	79.788	23.797	-5.813	1.00 20.00	6
	ATOM	1130	NZ	LYS	В	207	78.695	23.557	-6.791	1.00 20.00	7
	ATOM	1131	C	LYS	В	207	83.657	21.808	-2.487	1.00 20.00	6
	MOTA	1132	0	LYS	В	207	84.416	22.656	-2.960	1.00 20.00	8
	ATOM	1133	N	PRO	В	208	83.916	20.494	-2.582	1.00 20.00	7
45	ATOM	1134	CD	PRO	В	208	83.153	19.378	-1.993	1.00 20.00	6
	ATOM	1135	CA	PRO	В	208	85.122	20.005	-3.259	1.00 20.00	6
	ATOM	1136	CB	PRO	В	208	84.922	18.494	-3.267	1.00 20.00	6
	MOTA	1137	CG	PRO	В	208	84.174	18.256	-1.984	1.00 20.00	6
	MOTA	1138	C	PRO	В	208	85.303	20.574	-4.666	1.00 20.00	6
50	MOTA	1139	0	PRO	В	208	86.431	20.752	-5.124	1.00 20.00	8
	ATOM	1140	N	GLU	В	209	84.197	20.859	-5.347	1.00 20.00	7
	MOTA	1141	CA			209	84.243	21.410	-6.705	1.00 20.00	6
	ATOM	1142	СВ			209	82.836	21.424	-7.317	1.00 20.00	6
	ATOM	1143	CG			209	82.755	22.081	-8.690	1.00 20.00	6
55	ATOM	1144	CD			209	81.323	22.296	-9.159	1.00 20.00	6
	ATOM	1145	0E1			209	80.587	21.299	-9.322	1.00 20.00	8
	ATOM	1146		GLU			80.933	23.465	-9.364	1.00 20.00	8
	ATOM	1147	C			209	84.810	22.836	-6.716	1.00 20.00	6
	MOTA	1148	ō			209	85.409	23.269	-7.705	1.00 20.00	8

	MOTA	1149	N	ASN :	B 2	210		84.604	23.549	-5.612	1.00 20.00	7
	MOTA	1150	CA	ASN :	B 2	210		85.051	24.932	-5.439	1.00 20.00	6
	ATOM	1151	CB	ASN :	в 2	210		84.033	25.695	-4.588	1.00 20.00	6
	ATOM	1152	CG	ASN	в 2	210		82.851	26.170	-5.396	1.00 20.00	6
5	ATOM	1153	OD1	ASN	B 2	210		81.807	26.520	-4.846	1.00 20.00	8
	ATOM	1154	ND2	ASN	B 2	210		83.010	26.194	-6.717	1.00 20.00.	7
	ATOM	1155	C ·	ASN	в 2	210		86.427	25.070	-4.797	1.00 20.00	6
	ATOM	1156	0	ASN	В 2	210		86.937	26.181	-4.641	1.00 20.00	8
	MOTA	1157	N	ILE	в 2	211		87.016	23.948	-4.406	1.00 20.00	7
10	ATOM	1158	CA	ILE	в :	211		88.331	23.958	-3.790	1.00 20.00	6
	ATOM	1159	CB	ILE				88.336	23.090	-2.521	1.00 20.00	6
	ATOM	1160		ILE	в :	211		89.732	23.025	-1.925	1.00 20.00	6
	MOTA	1161	CG1	ILE	в :	211		87.350	23.682	-1.510	1.00 20.00	6
	ATOM	1162		ILE	в :	211		87.121	22.832	-0.285	1.00 20.00	6
15	ATOM	1163	C	ILE	в :	211		89.307	23.414	-4.816	1.00 20.00	6
	ATOM	1164	Ō	ILE				89.475	22.199	-4.949	1.00 20.00	8
	ATOM	1165	N	LEU				89.938	24.319	-5.558	1.00 20.00	7
	ATOM	1166	CA	LEU				90.875	23.918	-6.601	1.00 20.00	6
	ATOM	1167	СВ	LEU				90.966	25.012	-7.673	1.00 20.00	6
20	MOTA	1168	CG	LEU				89.630	25.510	-8.235	1.00 20.00	6
20	ATOM	1169		LEU				89.896	26.462	-9.390	1.00 20.00	6
	ATOM	1170		LEU				88.781	24.331	-8.709	1.00 20.00	6
	ATOM	1171	C	LEU				92.254	23.628	-6.038	1.00 20.00	6
	ATOM	1172	ō	PEA				92.537	23.923	-4.873	1.00 20.00	8
25	MOTA	1173	N	LEU				93.114	23.053	-6.875	1.00 20.00	7
23	ATOM	1174	CA	LEU				94.472	22.714	-6.472	1.00 20.00	6
	ATOM	1175	CB	LEU				94.609	21.192	-6.388	1.00 20.00	6
	ATOM	1176	CG	LEU				93.775	20.526	-5.292	1.00 20.00	6
	ATOM	1177		LEU				93.737	19.035	-5.508	1.00 20.00	6
30	ATOM	1178		LEU				94.374	20.852	-3.935	1.00 20.00	6
50 .	ATOM	1179	C	LEU				95.503	23.277	-7.449	1.00 20.00	6
	ATOM	1180	Ö	LEU				95.422	23.033	-8.657	1.00 20.00	8
	ATOM	1181				214 ·		96.470	24.036	-6.940	1.00 20.00	7
	ATOM	1182	CA	ASN				97.488	24.585	-7.826	1.00 20.00	6
35	ATOM	1183	CB	ASN				98.198	25.792	-7.201	1.00 20.00	6
55	ATOM	1184	CG	ASN			•	98.938	25.448	-5.927	1.00 20.00	6
	ATOM	1185		ASN				99.267	24.288	-5.669	1.00 20.00	8
	ATOM	1186		ASN				99.224	26.469	-5.123	1.00 20.00	7
	ATOM	1187	C	ASN				98.508	23.515	-8.182	1.00 20.00	6
40	ATOM	1188	ō	ASN				98.420	22.372	-7.725	1.00 20.00	8
40	ATOM	1189	N	GLU				99.482	23.894	-8.996	1.00 20.00	7
	ATOM	1190	CA	GLU				100.514	22.965	-9.430	1.00 20.00	6
	ATOM	1191	CB	GLU		215		101.491	23.687	-10.362	1.00 20.00	6
	ATOM	1192	CG	GLU				102.544		-10.979	1.00 20.00	6
45	ATOM	1193	CD	GLU				103.323	23.482	-12.080	1.00 20.00	6
43	ATOM	1194		GLU				103.909		-11.810	1.00 20.00	8
	MOTA	1195		GLU				103.344		-13.215	1.00 20.00	8
	ATOM	1196	C	GLU				101.275	22.307	-8.274	1.00 20.00	6
	ATOM	1197	0	GLU				101.801	21.205	-8.428	1.00 20.00	8
50	ATOM	1198	N	ASP				101.335	22.976	-7.123	1.00 20.00	7
50	MOTA	1199	CA	ASP	В	216 `		102.036	22.430	-5.958	1.00 20.00	6
	ATOM	1200	CB	VGD	B	216		102.727	23.549	-5.179	1.00 20.00	6
		1200	CG			216		103.952	24.086	-5.896	1.00 20.00	6
	ATOM ATOM	1201		ASP				104.766	23.267	-6.376	1.00 20.00	8
55	ATOM	1202		ASP				104.700	25.323	-5.973	1.00 20.00	8
55	ATOM	1203	C			216		101.121	21.651	-5.013	1.00 20.00	6
	ATOM		0			216		101.532	21.241	-3.925	1.00 20.00	
		1205	N			217		99.877	21.463	-5.434	1:00 20.00	
	MOTA	1206				217		98.890	20.730	-4.657	1.00 20.00	
	MOTA	1207	CA	PIE I	2	٠		20.020				

	ATOM	1208	CB	MET I	3 217	99.402	19.319	-4.358	1.00 20.00	6
	ATOM	1209	CG	MET I	3 217	99.456	18.432	-5.601	1.00 20.00	6
	ATOM	1210	SD	MET I	3 217	97.857	18.342	-6.445	1.00 20.00	16
	ATOM	1211	CE	MET 1	3 217	97.073	16.984	-5.543	1.00 20.00	6
5	ATOM	1212	'C	MET 1	3 217	98.397	21.403	-3.373	1.00 20.00	6
	ATOM	1213	0	MET I	3 217	97.972	20.730	-2.435	1.00 20.00	8
	MOTA	1214	N	HIS 1	B 218	98.469	22.730	-3.331	1.00 20.00	7
	ATOM	1215	CA		B 218	97.949	23.487	-2.197	1.00 20.00	6
	ATOM	1216	CB		B 218	98.831	24.700	-1.898	1.00 20.00	6
10	ATOM	1217	CG		B 218	100.100	24.357	-1.177	1.00 20.00	6
10		1218			B 218	101.390	24.362	-1.588	1.00 20.00	6
	MOTA	1219			B 218	100.117	23.935	0.136	1.00 20.00	7
	MOTA				B 218	101.364	23.698	0.504	1.00 20.00	6
	ATOM	1220			B 218	102.156	23.947	-0.524	1.00 20.00	7
1.5	MOTA	1221			B 218	96.583	23.939	-2.703	1.00 20.00	6
15	MOTA	1222	C			96.400	24.090	-3.910	1.00 20.00	8
	ATOM	1223	0		B 218		24.160	-1.808	1.00 20.00	7
	MOTA	1224	N		B 219			-2.257	1.00 20.00	6
	MOTA	1225	CA		B 219		24.562		1.00 20.00	6
	ATOM	1226	CB		B 219		24.359	-1.159		6
20	MOTA	1227			B 219		22.918	-0.654	1.00 20.00	
	ATOM	1228	CG1		B 219		25.353	-0.011	1.00 20.00	6
	ATOM	1229	CD1		B 219		25.342	1.036	1.00 20.00	6
	MOTA	1230	С		B 219		26.010	-2.714	1.00 20.00	6
	ATOM	1231	0		B 219		26.850	-2.375	1.00 20.00	8
25	ATOM	1232	N	GLN	B 220	93.168	26.274	-3.497	1.00 20.00	7
	ATOM	1233	CA	GLN	B 220	92.859	27.600	-3.999	1.00 20.00	6
	MOTA	1234	CB	GLN	B 220	93.537	27.867	-5.350	1.00 20.00	6
	MOTA	1235	CG	GLN	B 220	95.011	28.246	-5.216	1.00 20.00	6
	ATOM	1236	$^{\rm CD}$	GLN	B 220	95.599	28.799	-6.503	1.00 20.00	6
30	MOTA	1237	OE1	GLN	B 220	95.725	28.086	-7.502	1.00 20.00	8
	ATOM	1238	NE2	GLN	B 220	95.957	30.079	-6.486	1.00 20.00	7
	ATOM	1239	C		B 220		27.626	-4.140	1.00 20.00	6
	ATOM	1240	0	GLN	B 220	90.792	27.133	-5.124	1.00 20.00	8
	ATOM	1241	N		B 221		28.178	-3.129	1.00 20.00	7
35	ATOM	1242	CA		B 221		28.260	-3.122	1.00 20.00	б
55	ATOM	1243	CB		B 221		28.550	-1.700	1.00 20.00	6
	ATOM	1244	CG2		B 221		28.707	-1.708	.1.00 20.00	6
	ATOM	1245			B 221		27.406	-0.773	1.00 20.00	6
	ATOM	1245			B 221		27.559	0.668	1.00 20.00	6
40		1247	CDI		B 223		29.339	-4.092	1.00 20.00	6
40	ATOM		0		B 22:		30.374	-4.262	1.00 20.00	8
	MOTA	1248			B 222		29.082	-4.748	1.00 20.00	7
	ATOM	1249	N CA		B 222		30.039	-5.701	1.00 20.00	6
	ATOM	1250			B 222	,	29.728	-7.125	1.00 20.00	6
	MOTA	1251	CB		B 222				1.00 20.00	8
45	ATOM	1252	OG1					-7.618	1.00 20.00	6
	ATOM	1253			B 223		28.410	-5.683	1.00 20.00	6
	ATOM	1254	C		B 223		30.028		1.00 20.00	8
•	MOTA	1255	0		B 22:		29.417	-4.791	1.00 20.00	7
	MOTA	1256	N		B 22		30.712	-6.659	1.00 20.00	6
50	MOTA	1257	CA		B 22		30.806	-6:806		6
	MOTA	1258	CB		B 22		29.399	-6.767	1.00 20.00	
	MOTA	1259	CG		B 22		29.384	-7.205	1.00 20.00	6 8
	MOTA	1260			B 22		30.335	-7.900	1.00 20.00	_
	MOTA	1261	OD2		B 22		28.414	-6.866	1.00 20.00	
55	ATOM	1262	С		B 22		31.694	-5.725	1.00 20.00	
	MOTA	1263	0		B 22		31.208	-4.820	1.00 20.00	
	MOTA	1264	N		B 22		33.001	-5.848	1.00 20.00	
	MOTA	1265	CA		B 22		33.970	-4.866	1.00 20.00	
	MOTA	1266	CB	PHE	B. 22	4 83.800	34.869	-4.451	1.00 20.00	6

	ATOM	1267	CG	PHE	В	224		84.826	34.165	-3.612	1.00 20.00	6
	ATOM	1268	CD1	PHE	В	224	•	84.590	33.931	-2.261	1.00 20.00	6
	ATOM	1269	CD2	PHE	В	224		86.001	33.687	-4.182	1.00 20.00	6
	ATOM	1270	CE1	PHE	В	224		85.509	33.227	-1.486	1.00 20.00	6
5	ATOM	1271		PHE				86.927	32.981	-3.418	1.00 20.00	6
_	ATOM	1272	CZ	PHE				86.679	32.750	-2.068	1.00 20.00	6
	ATOM	1273	C	PHE				81.443	34.839	-5.256	1.00 20.00	6
	ATOM	1274	Ö	PHE				81.001	35.678	-4.468	1.00 20.00	8
			И.	GLY				80.928	34.647	-6.463	1.00 20.00	7
10	ATOM	1275										
10	MOTA	1276	CA	GLY				79.793	35.438	-6.894	1.00 20.00	6
	MOTA	1277	С	GLY				78.612	35.265	-5.955	1.00 20.00	6
	MOTA	1278	0	GLY				77.824	36.192	-5.753	1.00 20.00	8
	ATOM	1279	N	THR				78.486	34.080	-5.367	1.00 20.00	7
	ATOM	1280	CA	THR				77.379	33.819	-4.459	1.00 20.00	6
15	ATOM	1281	CB	THR	В	226		76.779	32.425	-4.715	1.00 20.00	6
	ATOM	1282	OG1	THR	В	226		77.826	31.450	-4.762	1.00 20.00	8
	MOTA	1283	CG2	THR	В	226		76.021	32.417	-6.041	1.00 20.00	6
	MOTA	1284	C	THR	В	226		77.738	33.957	-2.981	1.00 20.00	6
	MOTA	1285	0	THR	В	226		77.001	33.500	-2.107	1.00 20.00	8
20	MOTA	1286	N	ALA	В	227		78.867	34.598	-2.702	1.00 20.00	7
	ATOM	1287	CA	ALA	В	227		79.282	34.800	-1.325	1.00 20.00	6
	ATOM	1288	CB	ALA				80.738	35.242	-1.268	1.00 20.00	6
	ATOM	1289	C	ALA				78.384	35.875	-0.726	1.00 20.00	6
	ATOM	1290	ō	ALA				77.623	36.529	-1.440	1.00 20.00	8
25	ATOM	1291	И.	LYS				78.467	36.046	0.586	1.00 20.00	7
23		1291	CA	LYS				77.670	37.051	1.274	1.00 20.00	6
	ATOM		CB	LYS	_			76.637	36.384	2.179	1.00 20.00	6
	ATOM	1293	_									6
	MOTA	1294	CG	LYS				75.705	37.357	2.890	1.00 20.00	
20	ATOM	1295	CD	LYS		228		74.795	38.072	1.893	1.00 20.00	6
30	ATOM	1296	CE	LYS				73.849	39.049	2.587	1.00 20.00	6
	MOTA	1297	NZ	LYS				73.000	39.781	1.605	1.00 20.00	7
	ATOM	1298	С	LYS		228		78.616	37.896	2.110	1.00 20.00	6
	MOTA	-1299	0	LYS	В	228		79.355	37.366	2.940	1.00 20.00	8
	ATOM	1300	N	VAL	В	229		78.603	39.206	1.881	1.00 20.00	7
35	ATOM	1301	CA	VAL	В	229		79.463	40.114	2.626	1.00 20.00	6
	ATOM	1302	CB	VAL	В	229		79.976	41.256	1.734	1.00 20.00	6
	ATOM	1303	CG1	VAL	В	229		80.853	42.191	2.540	1.00 20.00	6
	ATOM	1304	CG2	VAL	В	229		80.746	40.686	0.561	1.00 20.00	6
	ATOM	1305	C	VAL	В	229		78.687	40.710	3.793	1.00 20.00	6
40	ATOM	1306	0	VAL	В	229		77.798	41.537	3.599	1.00 20.00	8
	ATOM	1307	N	LEU	В	230		79.034	40.284	5.003	1.00 20.00	7
	ATOM	1308	CA	LEU	В	230		78.370	40.752	6.213	1.00 20.00	6
	ATOM	1309	CB	LEU	В	230		78.740	39.856	7.395	1.00 20.00	6
	ATOM	1310	CG	LEU	В	230		78.276	38.403	7.332	1.00 20.00	6
45	ATOM	1311		LEU				78.853	37.634	8.508	1.00 20.00	6
73	ATOM	1312		LEU				76.760	38.350	7.339	1.00 20.00	6
	ATOM	1312	CDZ	LEU				78.705	42.193	6.565	1.00 20.00	6
											1.00 20.00	8
	ATOM	1314	0	LEU				79.768	42.701	6.214		
	ATOM	1315	N	SER				77.781	42.839	7.270	1.00 20.00	7
50	ATOM	1316	CA	SER				77.957	44.219	7.708	1.00 20.00	6
	MOTA	1317	CB			231		77.082	45.161	6.875	1.00 20.00	6
	ATOM	1318	OG	SER				75.714	44.795	6.948	1.00 20.00	8
	MOTA	1319	С	SER				77.623	44.373	9.196	1.00 20.00	6
	MOTA	1320	0	SER				78.322	45.086	9.919	1.00 20.00	8
55	MOTA	1321	N	PRO				76.553	43.705	9.674	1.00 20.00	7
	ATOM	1322	CD			232		75.571	42.876	8.948	1.00 20.00	6
	ATOM	1323	CA			232		76.182	43.811	11.091	1.00 20.00	6
	MOTA	1324	CB	PRO	В	232		75.005	42.844	11.211	1.00 20.00	6
	MOTA	1325	CG	PRO	В	232		74.367	42.933	9.862	1.00 20.00	. 6

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	ATOM	1326	С	PRO B	232	77.332	43.438	12.024	1.00 20.00	6
	ATOM	1327	0	PRO B	232	78.199	42.640	11.666	1.00 20.00	8
	ATOM	1328	N	ALA B	237	74.215	38.132	11.762	1.00 20.00	7
	MOTA	1329	CA	ALA B	237	74.666	37.653	10.460	1.00 20.00	6
5	ATOM	1330	CB	ALA B	237	75.541	36.417	10.637	1.00 20.00	6
	MOTA	1331	С	ALA B	237	73.479	37.324	9.558	1.00 20.00	6
	MOTA	1332	0	ALA B	237	73.143	36.158	9.374	1.00 20.00	8
	MOTA	1333	N	ALA B	238	72.841	38.347	8.996	1.00 20.00	7
	ATOM	1334	CA	ALA B	238	71.693	38.130	8.117	1.00 20.00	6
10	MOTA	1335	CB	ALA B		70.973	39.450	7.853	1.00 20.00	6
	MOTA	1336	C	ALA B	238	72'. 123	37.497	6.798	1.00 20.00	6
	MOTA	1337	0	ALA B		73.315	37.404	6.500	1.00 20.00	8
	MOTA	1338	N	ALA B		71.146	37.057	6.012	1.00 20.00	7
	MOTA	1339	CA	ALA B		71.439	36.431	4.728	1.00 20.00	6
15	MOTA	1340	CB	ALA B		72.152	35.123	4.952	1.00 20.00	6
	MOTA	1341	C	ALA B		70.173	36.194	3.918	1.00 20.00	6
	MOTA	1342	0	ALA B		69.329	37.079	3.825	1.00 20.00	8
	MOTA	1343	N	ASN B		70.068	34.996	3.339	1.00 20.00	7
	MOTA	1344	CA	ASN E		68.939	34.559	2.514	1.00 20.00	6
20	MOTA	1345	CB	ASN E		67.614	35.160	2.999	1.00 20.00	6
	MOTA	1346	CG	ASN E		67.258	36.466	2.299	1.00 20.00	6
	MOTA	1347		ASN E		67.119	36.519	1.068	1.00 20.00	8
	MOTA	1348		ASN E		67.091	37.536	3.089	1.00 20.00	7
	MOTA	1349	C	ASN E		69.153	34.937	1.053	1.00 20.00	6
25	MOTA	1350.	0	ASN E		70.007	35.767	0.749	1.00 20.00	8
	ATOM	1351	N	ALA E		68.365	34.329	0.163	1.00 20.00	7
	ATOM	1352	CA	ALA E		68.401	34.570	-1.290	1.00 20.00	6
	ATOM	1353	C	ALA E		68.990	33.416	-2.103	1.00 20.00	6 8
	MOTA	1354	0	ALA E		68.353	32.919	-3.030	1.00 20.00 1.00 20.00	6
30	ATOM	1355	CB	ALA E		69.168	35.859	-1.629	1.00 20.00	7
	ATOM	1356	N	PHE E		70.205	33.000	-1.762 -2.481	1.00 20.00	6
	MOTA	1357	CA	PHE E		70.875	31.918 32.379	-2.952	1.00 20.00	6
	ATOM	1358	CB	PHE E		72.259 73.102	31.273	-3.521	1.00 20.00	6
35	ATOM	1359	CG	PHE E		72.843	30.767	-4.790	1.00 20.00	6
33	ATOM	1360		PHE E		74.136	30.707	-2.773	1.00 20.00	6
	MOTA	1361		PHE E		73.599	29.718	-5.310	1.00 20.00	6
	ATOM	1362 1363	CE2	PHE E		74.896	29.666	-3.281	1.00 20.00	6
	ATOM ATOM	1364	CZ	PHE		74.627	29.166	-4.553	1.00 20.00	6
40	ATOM	1365	C	PHE E		71.038	30.652	-1.646	1.00 20.00	6
40	ATOM	1366	0	PHE E		71.213	30.716	-0.431	1.00 20.00	8
	ATOM	1367	N	VAL E		70.988	29.505	-2.318	1.00 20.00	7
	MOTA	1368	CA	VAL E		71.157	28.204	-1.675	1.00 20.00	6
	ATOM	1369	CB	VAL E		69.828	27.420	-1.617	1.00 20.00	6
45	ATOM	1370		VAL E		70.066	26.023	-1.050	1.00 20.00	б
43	ATOM	1371		VAL E		68.825	28.177	-0.766	1.00 20.00	6
	ATOM	1372	C	VAL E		72.164	27.394	-2.486	1.00 20.00	6
	ATOM	1373	ō	VAL E		71.894	27.014	-3.628	1.00 20.00	8
	MOTA	1374	N	GLY E		73.323	27.137	-1.890	1.00 20.00	7
50	ATOM	1375	CA	GLY H		74.364	26.385	-2.569	1.00 20.00	6
	ATOM	1376	C	GLY F		74.019	24.944	-2.911	1.00 20.00	6
	ATOM	1377	0	GLY E		72.867	24.524	-2.810	1.00 20.00	8
	ATOM	1378	N	THR I		75.032	24.184	-3.315	1.00 20.00	7
	ATOM	1379	CA	THR I		74.858	22.787	-3.691	1.00 20.00	6
55	ATOM	1380	CB	THR I		76.214	22.161	-4.046	1.00 20.00	6
	ATOM	1381	OG1	THR I	245	76.794	22.911	-5.120	1.00 20.00	8
	ATOM	1382	CG2	THR I	3 245	76.049	20.710	-4.485	1.00 20.00	6
	MOTA	1383	C	THR I	3 245	74.174	22.003	-2.579	1.00 20.00	6
	ATOM	1384	0	THR I	3 245	74.643	21.969	-1.441	1.00 20.00	8

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	MOTA	1385	N	аца в	246	73.061	21.372	-2.937	1.00 20.00	7
	MOTA	1386	CA	ALA B	246	72.229	20.615	-2.008	1.00 20.00	6
	MOTA	1387	CB	ALA B	246	71.266	19.723	-2.793	1.00 20.00	6
	MOTA	1388	С	ALA B	246	72.936	19.789	-0.941	1.00 20.00	6
5	ATOM	1389	0	ALA B	246	72.611	19.894	0.239	1.00 20.00	8
	ATOM	1390	N	GLN B	247	73.902	18.973	-1.339	1.00 20.00	7
	MOTA	1391	CA	GLN E	247	74.580	18.121	-0.371	1.00 20.00	6
	ATOM	1392	CB	GLN B	247	75.535	17.168	-1.096	1.00 20.00	6
	ATOM	1393	CG	GLN B	247	75.110	16.823	-2.520	1.00 20.00	6
10	ATOM	1394	CD	GLN E	3 247	75.139	15.336	-2.811	1.00 20.00	6
••	ATOM	1395	OE1	GLN E	3 247	75.963	14.602	-2.270	1.00 20.00	8
	ATOM	1396		GLN E		74.246	14.887	-3.686	1.00 20.00	7
	ATOM	1397	C	GLN E		75.343	18.873	0.720	1.00 20.00	6
	ATOM	1398	0	GLN E	3 247	75.631	18.306	1.773	1.00 20.00	8
15	ATOM	1399	N	TYR E	3 248	75.648	20.147	0.484	1.00 20.00	7
••	MOTA	1400	CA	TYR E		76.405	20.941	1.454	1.00 20.00	6
	ATOM	1401	СВ	TYR F		77.642	21.531	0.767	1.00 20.00	6
	ATOM	1402	CG	TYR F		78.447	20.471	0.052	1.00 20.00	6
	ATOM	1403			3 248	79.329	19.648	0.750	1.00 20.00	6
20	ATOM	1404		TYR I		79.979	18.589	0.115	1.00 20.00	6
20	ATOM	1405	CD2	TYR I		78.243	20.220	-1.306	1.00 20.00	6
	ATOM	1406	CE2	TYR I		78.884	19.167	-1.951	1.00 20.00	6
	MOTA	1407	CZ		3 248	79.748	18.352	-1.232	1.00 20.00	б
	MOTA	1408	ОН	TYR I		80.348	17.280	-1.852	1.00 20.00	8
25	MOTA	1409	C	TYR I		75.596	22.055	2.118	1.00 20.00	6
	ATOM	1410	0	TYR I	B 248	76.132	22.824	2.917	1.00 20.00	8
	ATOM	1411	N		B 249	74.309	22.135	1.798	1.00 20.00	7
	ATOM	1412	CA		B 249	73.452	23.162	2.376	1.00 20.00	6
	MOTA	1413	CB	VAL 3	B 249	72.071	23.174	1.695	1.00 20.00	6
30	ATOM	1414	CG1	VAL I	B 249	71.117	24.100	2.442	1.00 20.00	6
50	ATOM	1415		VAL :		72.225	23.632	0.264	1.00 20.00	6
	ATOM	1416	С		B 249	73.262	22.964	3.875	1.00 20.00	6
	ATOM	1417	0	VAL	B 249	73.027	21.847	4.341	1.00 20.00	8
	MOTA	1418	N	SER	В 250	73.373	24.055	4.628	1.00 20.00	7
35	ATOM	1419	CA	SER	B 250	73.206	24.008	6.076	1.00 20.00	6
	MOTA	1420	CB	SER	B 250	73.921	25.198	6.738	1.00 20.00	6
	ATOM	1421	OG	SER	B 250	73.428	26.440	6.257	1.00 20.00	8
	MOTA	1422	С	SER	B 250	71.717	24.049	6.405	1.00 20.00	6
	ATOM -	1423	0	SER	B 250	70.920	24.577	5.636	1.00 20.00	8
40	MOTA	1424	N	PRO	B 251	71.322	23.479	7.550	1.00 20.00	7
	MOTA	1425	CD	PRO	B 251	72.130	22.770	8.558	1.00 20.00	6
	MOTA	1426	CA	PRO	B 251	69.905	23.484	7.925	1.00 20.00	. 6
	MOTA	1427	CB	PRO	B 251	69.892	22.714	9.252	1.00 20.00	6 6
	ATOM	1428	. CG	PRO	B 251	71.290	22.936	9.801	1.00 20.00	6
45	ATOM	1429	С		B 251	69.265	24.870	8.032	1.00 20.00	8
	ATOM	1430	0	PRO	B 251	68.093	25.036	7.688	1.00 20.00	7
	MOTA	1431	N		B 252	70.017	25.867	8.492	1.00 20.00 1.00 20.00	6
	MOTA	1432	CA		B 252	69.462	27.216	8.625		6
	MOTA	1433	CB		B 252	70.503	28.193	9.196		6
50	MOTA	1434	CG		B 252	71.838	28.180	8.477		6
	MOTA	1435	CD		B 252	72.844	27.257	9.139		8
	MOTA	1436			B 252	72.429	26.207	9.675		8
	MOTA	1437			B 252	74.053	27.581	9.118		
	MOTA	1438	С		B 252	68.928		7.292 7.261		
55	MOTA	1439	0		B 252	67.927		6.189		
	ATOM	1440	N		B 253	69.584 69.117		4.883		
	MOTA	1441			B 253	70.140		3.794		
	MOTA	1442			B 253	70.140		3.421		
	ATOM	1443	CG	LEU	B 253	/1.14/	20.033	J. 461		

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	ATOM	1444	CD1	LEU	В	253	72.12	L 28.851	4.547	1.00 20.00	6
	ATOM	1445	CD2	TEU	В	253	71.858	3 28.250	2.140	1.00 20.00	6
	MOTA	1446	С	LEU	В	253	67.77	27.227	4.496	1.00 20.00	6
	MOTA	1447	0 -	LEU	В	253	66.99	7 27.826	3.751	1.00 20.00	8
5	MOTA	1448	N	LEU	В	254	67.50	26.029	5.002	1.00 20.00	7
	ATOM	1449	CA	LEU	В	254	66.27	25.316	4.689	1.00 20.00	6
	MOTA	1450	CB	LEU	В	254	66.539	23.809	4.689	1.00 20.00	6
	ATOM	1451	CG	LEU	В	254	67.64	7 23.322	3.746	1.00 20.00	6
	ATOM	1452	CD1	LEU	В	254	67.983	3 21.873	4.057	1.00 20.00	6
10	MOTA	1453	CD2	LEU	В	254	67.204	23.475	2.302	1.00 20.00	6
	ATOM	1454	C	LEU	В	254	65.135	25.626	5.662	1.00 20.00	6
	MOTA	1455	0	LEU	В	254	63.959	25.524	5.312	1.00 20.00	8
	MOTA	1456	N	THR	В	255	65.483	26.010	6.883	1.00 20.00	7
	MOTA	1457	CA	THR	В	255	64.472	26.308	7.884	1.00 20.00	6
15	MOTA	1458	CB	THR	В	255	64.876	25.747	9.252	1.00 20.00	6
	MOTA	1459	OG1	THR	В	255	66.154	26.277	9.619	1.00 20.00	8
	ATOM	1460	CG2	THR			64.958	3 24.230	9.202	1.00 20.00	6
	MOTA	1461	C	THR	В	255	64.209	27.795	8.035	1.00 20.00	6
	MOTA	1462	0	THR	В	255	63.072	28.241	7.897	1.00 20.00	8
20	MOTA	1463	N	GLU	В	256	65.250	28.560	8.314	1.00 20.00	7
	MOTA	1464	CA	GLU	В	256	65.115	30.001	8.507	1.00 20.00	6
	MOTA	1465	CB	GLU			66.01	30.444	9.659	1.00 20.00	
	MOTA	1466	CG	GLU	В	256	65.634	29.818	10.987	1.00 20.00	
	MOTA	1467	CD	GLU			66.73		12.018	1.00 20.00	
25	MOTA	1468		GLU			67.249		12.232	1.00 20.00	
	ATOM	1469	OE2	GLU			67.086		12.619	1.00 20.00	
	ATOM	1470	C	GLU			65.439		7.262	1.00 20.00	
	ATOM	1471	0	GLU			65.268		7.252	1.00 20.00	
	MOTA	1472	N	LYS			65.90		6.215	1.00 20.00	
30	MOTA	1473	CA	LYS			66.260		4.970	1.00 20.00	
	ATOM	1474	CB	LYS			65.01		4.352	1.00 20.00	
	MOTA	1475	CG	LYS		257	65.184		2.915	1.00 20.00	
	ATOM	1476	CD	LYS			63.885		2.378	1.00 20.00	
2.5	MOTA	1477	CE	LYS			63.994		0.902	1.00 20.00	
35	MOTA	1478	NZ	LYS			65.060		0.640	1.00 20.00	
	MOTA	1479	C	LYS			67.309		5.263	1.00 20.00	
	ATOM	1480	0	LYS			67.270			1.00 20.00	
	ATOM	1481 1482	n Ca	SER SER			68.243 69.30		6.152 6.527	1.00 20.00	
40	ATOM		CB	SER			69.043		7.937	1.00 20.00	
40	ATOM ATOM	1483 1484	OG	SER			68.893		8.859	1.00 20.00	
	ATOM	1485	C	SER			70.67		6.467	1.00 20.00	
	ATOM	1486	Ö	SER			70.786		6.542	1.00 20.00	
	ATOM	1487	N	ALA			71.718		6.329	1.00 20.00	
45	ATOM	1488	CĄ	ALA			73.08		6.252	1.00 20.00	6
	ATOM	1489	CB	ALA			73.549		4.809	1.00 20.00	
,	ATOM	1490	C	ALA			74.03		7.102	1.00 20.00	
	ATOM	1491	Ö	ALA			73.882		7.211	1.00 20.00	
	ATOM	1492	N	CYS			75.008		7.704	1.00 20.00	
50	ATOM	1493	CA	CYS			75.99		8.550	1.00 20.00	
-	ATOM	1494	CB	CYS			75.57	•	10.017	1.00 20.00	
	ATOM	1495	SG	CYS			75.30		10.594	1.00 20.00	
	ATOM	1496	С	CYS			77.328		8.349	1.00 20.00	
	MOTA	1497	ō	CYS			77.410		7.620	1.00 20.00	
55	ATOM	1498	N	LYS			78.37		8.993	1.00 20.00	
	ATOM	1499	CA	LYS			79.69		8.869	1.00 20.00	
	ATOM	1500	CB	LYS			80.67		9.821	1.00 20.00	6
	ATOM	1501	CG	LYS			80.98		9.472	1.00 20.00	
	ATOM	1502	CD	LYS			81.96		10.475	1.00 20.00	
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	ATOM	1503	CE	LYS	В	261	82.157	36.365	10.259	1.00	20.00	6
	ATOM	1504	NZ	LYS	В	261	83.085	36.922	11.278	1.00	20.00	7
	ATOM	1505	C	LYS	В	261	79.632	30.687	9.187		20.00	6
	ATOM	1506	ō	LYS			80.258	29.877	8.512		20.00	8
· 5	ATOM	1507	N	SER			78.860	30.346	10.214		20.00	7
,	ATOM	1508	CA	SER				28.966	10.659		20.00	6
			CB	SER			78.716					
	ATOM	1509					77.806	28.913	11.895		20.00	6
	ATOM	1510	OG	SER			77.884	27.657	12.546		20.00	8
	MOTA	1511	C	SER			78.161	28.070	9.549		20.00	6
10	MOTA	1512	0	SER			78.350	26.856	9.575		20.00	8
	ATOM	1513	N	SER	В	263	77.466	28.660	8.581	1.00	20.00	7
	MOTA	1514	CA	SER	В	263	76.938	27.870	7.472	1.00	20.00	6
	ATOM	1515	CB	SER	В	263	76.132	28.750	6.507	1.00	20.00	6
	ATOM	1516	OG	SER	В	263	75.011	29.329	7.156	1.00	20.00	8
15	MOTA	1517	С	SER	В	263	78.123	27.244	6.737	1.00	20.00	6
	ATOM	1518	0,	SER	В	263	78.038	26.108	6.273	1.00	20.00	8
	ATOM	1519	N	ASP	в	264	79.234	27.977	6.642	1.00	20.00	7
	ATOM	1520	CA	ASP			80.419	27.448	5.961		20.00	6
	ATOM	1521	CB	ASP			81.478	28.538	5.745		20.00	6
20	MOTA	1522	CG	ASP			81.091	29.539	4.673		20.00	6
20		1523		ASP			80.286	29.187	3.786		20.00	8
•	ATOM			ASP					4.704		20.00	8
	MOTA	1524					81.617	30.676				
	ATOM	1525	C	ASP			81.043	26.312	6.771		20.00	6
	MOTA	1526	0	ASP			81.586	25.365	6.201		20.00	8
25	MOTA	1527	Ŋ	LEU			80.971	26.415	8.099		20.00	7
	ATOM	1528	CA	LEU			81.532	25.390	8.974		20.00	6.
	MOTA	1529	CB	LEU			81.491	25.848	10.438		20.00	6
	ATOM	1530	CG	LEU			82.419	27.035	10.746		20.00	6
•	MOTA	1531	CD1	LEU	В	265	82.204	27.532	12.177	1.00	20.00	6
30	ATOM	1532	CD2	LEU	В	265	83.864	26.608	10.541	1.00	20.00	6
	ATOM	1533	С	LEU	В	265	80.750	24.094	8.800	1.00	20.00	6
	ATOM	1534	0	LEU	В	265	81.306	23.004	8.910	1.00	20.00	8
	ATOM	1535	N	TRP	В	266	79.454	24.208	8.530	1.00	20.00	7
	ATOM	1536	CA	TRP	в	266	78.646	23.017	8.309	1.00	20.00	6
35	ATOM	1537	СВ	TRP			77.167	23.384	8.148	1.00	20.00	6
	ATOM	1538	CG	TRP			76.310	22.245	7.646		20.00	6
	ATOM	1539	CD2	TRP			75.455	21.399	8.426		20.00	6
	ATOM	1540	CE2	TRP			74.881	20.455	7.542		20.00	6
	ATOM	1541	CE3	TRP			75.117	21.345	9.785		20.00	6
40	ATOM	1542		TRP			76.220	21.792	6.356		20.00	6
40		1543	NE1	TRP			75.365	20.719	6.288		20.00	7
	MOTA						73.988				20.00	6
	ATOM	1544	CZ2	TRP				19.466	7.975			6
	ATOM	1545	CZ3	TRP		266	74.227	20.359	10.216		20.00	
	ATOM	1546	CH2	TRP			73.674	19.434	9.310		20.00	6
45	MOTA	1547	С	TRP			79.169	22.356	7.038		20.00	6
	MOTA	1548	0	TRP			79.356	21.142	6.988		20.00	8
	MOTA	1549	N	ALA			79.411	23.164	6.011		20.00	7
	MOTA	1550	CA	ALA	В	267	79.930	22.646	4.751	1.00	20.00	6
	MOTA	1551	CB	ALA	В	267	80.089	23.772	3.746	1.00	20.00	6
50	MOTA	1552	C	ALA	В	267	81.277	21.976	5.016	1.00	20.00	6
	MOTA	1553	0	ALA	В	267	81.570	20.914	4.471	1.00	20.00	8
	MOTA	1554	N	LEU	В	268	82.091	22.596	5.864	1.00	20.00	7
	ATOM	1555	CA	LEU			83.393	22.030	6.209	1.00	20.00	6
	ATOM	1556	CB	LEU			84.092	22.898	7.264		20.00	б
55	ATOM	1557	CG	LEU			85.379	22.332	7.879		20.00	6
	MOTA	1558		LEU			86.442	22.192	6.803		20.00	6
	ATOM	1559		LEU			85.872	23.263	9.006		20.00	6
	MOTA	1560	CD2	LEU			83.193	20.617	6.753		20.00	6
	ATOM	1561	0	LEU			83.903	19.684	6.372		20.00	8
	MION	TOOT	0	T) C (D	200	55.503	19.004	0.3/2	±. 00		•

	MOTA	1562	N	GLY	В	269		82.220	20.463	7.645	1.00 20.00	7
	MOTA	1563	CA	GLY	В	269		81.947	19.156	8.217	1.00 20.00	6
	ATOM	1564	С	GLY	В	269		81.597	18.125	7.156	1.00 20.00	6
	ATOM	1565	0	GLY	В	269		82.025	16.971	7.239	1.00 20.00	8
5	ATOM	1566	N	CYS	В	270		80.819	18.530	6.155	1.00 20.00	7
	ATOM	1567	CA	CYS	В	270		80.445	17.613	5.083	1.00 20.00	6
	ATOM	1568	CB	CYS	В	270		79.413	18.255	4.148	1.00 20.00	6
	ATOM	1569	SG	CYS	В	270		77.824	18.654	4.905	1.00 20.00	16
	ATOM	1570	C	CYS				81.682	17.241	4.265	1.00 20.00	6
10	ATOM	1571	0	CYS				81.852	16.090	3.866	1.00 20.00	8
	ATOM	1572	N	ILE				82.541	18.226	4.012	1.00 20.00	7
	ATOM	1573	CA	ILE				83.751	18.000	3.229	1.00 20.00	6
	ATOM	1574	СВ	ILE				84.436	19.339	2.903	1.00 20.00	6
	ATOM	1575		ILE				85.784	19.098	2.227	1.00 20.00	6
15	ATOM	1576		ILE				83.508	20.171	2.007	1.00 20.00	6
13	ATOM	1577		ILE				83.962	21.607	1.815	1.00 20.00	6
		1578	C	ILE				84.729	17.063	3.934	1.00 20.00	6
	MOTA		0	ILE				85.300	16.174	3.304	1.00 20.00	8
	ATOM	1579		ILE				84.927	17.258	5.236	1.00 20.00	7
20	MOTA	1580	N	ILE				85.820	16.382	5.987	1.00 20.00	6
20	MOTA	1581	CA	ILE				85.902	16.790	7.471	1.00 20.00	6
	MOTA	1582	CB	ILE				86.623	15.703	8.277	1.00 20.00	6
	MOTA	1583		ILE				86.646	18.120	7.606	1.00 20.00	6
	MOTA	1584		ILE				86.553	18.723	9.011	1.00 20.00	6
25	MOTA	1585	CDI	ILE				85.274	14.957	5.901	1.00 20.00	6
25	ATOM	1586 1587	0 .	ILE				86.021	14.003	5.679	1.00 20.00	8
	ATOM ATOM	1588	N	TYR				83.964	14.822	6.072	1.00 20.00	7
		1589	CA	TYR				83.324	13.518	6.006	1.00 20.00	6
	ATOM ATOM	1590	CB	TYR				81.825	13.651	6.287	1.00 20.00	6
30	ATOM	1591	CG	TYR				81.064	12.340	6.250	1.00 20.00	6
50	ATOM	1592		TYR		273	-	80.806	11.690	5.041	1.00 20.00	6
	ATOM	1593	CE1					80.107	10.486	5.005	1.00 20.00	6
	ATOM	1594		TYR				80.601	11.750	7,427	1.00 20.00	6
	ATOM	1595		TYR				79.904	10.548	7.405	1.00 20.00	6
35	ATOM	1596	CZ	TYR				79.659	9.922	6.192	1.00 20.00	6
33	ATOM	1597	OH	TYR				78.971	8.736	6.174	1.00 20.00	8
	ATOM	1598	C	TYR				83.550	12.897	4.632	1.00 20.00	6
	ATOM	1599	ō	TYR		273		83.865	11.713	4.526	1.00 20.00	8
	ATOM	1600	N	GLN				83.402	13.705	3.586	1.00 20.00	7
40	ATOM	1601	CA	GLN		274		83.579	13.230	2.220	1.00 20.00	6
-10	ATOM	1602	CB	GLN		274		83.176	14.322	1.222	1.00 20.00	6
	. ATOM	1603	CG	GLN		274		83.149	13.857	-0.230	1.00 20.00	6
	ATOM	1604	CD	GLN		274		82.558	14.898	-1.169	1.00 20.00	6
	MOTA	1605		GLN				82.108	15.961	-0.736	1.00 20.00	8
45	ATOM	1606		GLN				82.548	14.591	-2.462	1.00 20.00	7
43	ATOM	1607	C			274		85.013	12.788	1.953	1.00 20.00	6
	ATOM	1608	Ö			274		85.239	11.818	1.233	1.00 20.00	8
•	ATOM	1609	N			275		85.981	13.498	2.528	1.00 20.00	7
	ATOM	1610		LEU				87.389	13.143	2.333	1.00 20.00	6
50	ATOM	1611	CB			275		88.311	14.194	2.971	1.00 20.00	6
50	ATOM	1612	CG			275		88.418	15.561	2.284	1.00 20.00	6
	ATOM	1613		LEU				89.325	16.481	3.088	1.00 20.00	6
	ATOM	1614		LEU				88.969	15.379	0.879	1.00 20.00	6
	ATOM	1615	C			275		87.697	11.779	2.940	1.00 20.00	6
55	ATOM	1616	Ö			275		88.430	10.981	2.354	1.00 20.00	8
,,	ATOM	1617	N			276		87.125	11.519	4.112	1.00 20.00	7
	ATOM	1618	CA			276		87.353	10.269	4.827	1.00 20.00	6
	ATOM	1619	CB			276		87.096	10.451	6.342	1.00 20.00	6
	MOTA	1620		VAL				87.376	9.148	7.082	1.00 20.00	6

	ATOM	1621	CG2	VAL	В	276		87.973	11.580	6.891	1.00 20.00	6
	MOTA	1622	C	VAL	В	276		86.504	9.089	4.336	1.00 20.00	6
	MOTA	1623	0	VAL	В	276		87.005	7.973	4.195	1.00 20.00	8
	MOTA	1624	N	ALA	В	277		85.222	9.337	4.090	1.00 20.00	7
5	MOTA	1625	CA	ALA	В	277		84.310	8.291	3.643	1.00 20.00	6
	ATOM	1626	CB	ALA	В	277		82.898	8.597	4.124	1.00 20.00	6
	ATOM	1627	С	ALA	В	277		84.315	8.115	2.130	1.00 20.00	6
	ATOM	1628	0	ALA	В	277		84.036	7.029	1.627	1.00 20.00	8
	ATOM	1629	N	GLY	В	278		84.632	9.180	1.405	1.00 20.00	7
10	ATOM	1630	CA	GLY	В	278		84.653	9.099	-0.041	1.00 20.00	6
	ATOM	1631	С	GLY	В	278		83.365	9.627	-0.644	1.00 20.00	6
	ATOM	1632	0	GLY	в	278		83.272	9.817	-1.860	1.00 20.00	8
	ATOM	1633	N	LEU	В	279		82.375	9.867	0.211	1.00 20.00	7
	ATOM	1634	CA	LEU	В	279		81.075	10.382	-0.219	1.00 20.00	6
15	ATOM	1635	CB	LEU				80.070	9.232	-0.375	1.00 20.00	6
	ATOM	1636	CG	LEU				80.342	8.114	-1.385	1.00 20.00	6
	ATOM	1637		LEU				79.311	7.009	-1.191	1.00 20.00	6
	ATOM	1638	CD2	LEU				80.291	8.660	-2.804	1.00 20.00	6
	ATOM	1639	C	LEU				80.522	11.369	0.812	1.00 20.00	6
20	ATOM	1640	ŏ	LEU				80.750	11.218	2.007	1.00 20.00	8
20	ATOM	1641	N	PRO				79.787	12.395	0.361	1.00 20.00	7
	ATOM	1642	CD	PRO				79.403	12.730	-1.020	1.00 20.00	6
	ATOM	1643	CA	PRO				79.230	13.361	1.314	1.00 20.00	6
	MOTA	1644	CB	PRO				78.569	14.397	0.407	1.00 20.00	6
25.	MOTA	1645	CG	PRO				78.191	13.598	-0.802	1.00 20.00	6
23.	MOTA	1646	C	PRO				78.242	12.662	2.262	1.00 20.00	6
	ATOM	1647	0	PRO				77.666	11.633	1.913	1.00 20.00	8
	ATOM	1648	N	PRO				78.035	13.220	3.470	1.00 20.00	7
	ATOM	1649	CD	PRO				78.571	14.535	3.859	1.00 20.00	6
30	MOTA	1650	CA	PRO				77.145	12.701	4.520	1.00 20.00	6
50	ATOM	1651	CB	PRO				77.262	13.746	5.634	1.00 20.00	6
	ATOM	1652	CG	PRO				78.546	14.450	5.344	1.00 20.00	6
	ATOM	1653	C	PRO				75.679	12.485	4.142	1.00 20.00	6
	ATOM	1654	ō	PRO			*	75.094	11.441	4.442	1.00 20.00	8
35	MOTA	1655	N	PHE				75.088	13.487	3.504	1.00 20.00	7
33	ATOM	1656	CA	PHE				73.686	13.427	3.123	1.00 20.00	6
	ATOM	1657	CB	PHE				73.006	14.734	3.531	1.00 20.00	6
	ATOM	1658	CG	PHE				73.300	15.146	4.947	1.00 20.00	6
	ATOM	1659		PHE				72.624	14.560	6.013	1.00 20.00	6
40	ATOM	1660		PHE				74.295	16.085	5.218	1.00 20.00	6
40	ATOM	1661		PHE				72.934	14.902	7.331	1.00 20.00	6
	ATOM	1662		PHE				74.613	16.433	6.530	1.00 20.00	6
	ATOM	1663	CZ	PHE		282		73.930	15.840	7.591	1.00 20.00	6
	ATOM	1664	C	PHE				73.527	13.191	1.628	1.00 20.00	6
45		1665	0	PHE				73.797	14.079	0.819	1.00 20.00	8
43	ATOM ATOM	1666	N	ARG				73.080	11.994	1.267	1.00 20.00	7
	ATOM	1667	CA	ARG				72.888	11.635	-0.134	1.00 20.00	6
	MOTA	1668	CB	ARG				73.931	10.598	-0.559	1.00 20.00	6
	ATOM	1669	CG	ARG				75.358	10.928	-0.151	1.00 20.00	6
50	ATOM	1670	CD			283		76.326	9.883	-0.687	1.00 20.00	6
50			NE	ARG				76.054	8.555	-0.142	1.00 20.00	. 7
	MOTA MOTA	1671 1672	CZ			283		76.404	8.159	1.077	1.00 20.00	6
				ARG				77.047	8.986	1.893	1.00 20.00	7
	ATOM	1673		ARG				76.108	6.933	1.484	1.00 20.00	7
55	ATOM	1674	NH2			283		71.493	11.046	-0.331	1.00 20.00	6
55	ATOM	1675				283		70.957	10.391	0.563	1.00 20.00	8
	ATOM	1676	O N			284		70.937	11.276	-1.502	1.00 20.00	7
	ATOM	1677	N			284		69.579	10.755	-1.796	1.00 20.00	6
	ATOM	1678	CA					68.532	11.484	-0.961	1.00 20.00	6
	ATOM	1679	CB	ALLA	0	284		00.332	TT.404	U. JUI		-

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	MOTA	1680	С	ALA			69.278	10.921	-3.273	1.00 20.00	6
	ATOM	1681	0	ALA	В	284	70.007	11.611	-3.984	1.00 20.00	8
	MOTA	1682	N	GLY	В	285	68.191	10.299	-3.722	1.00 20.00	7
	MOTA	1683	CA	GLY	В	285	67.807	10.360	-5.122	1.00 20.00	6
5	MOTA	1684	C	GLY	В	285	67.561	11.737	-5.707	1.00 20.00	6
	ATOM	1685	0	GLY	В	285	67.775	11.955	-6.899	1.00 20.00	8
	ATOM	1686	N	ASN			67.089	12.673	-4.892	1.00 20.00	7
		1687	CA	ASN			66.835	14.018	-5.386	1.00 20.00	6
	ATOM									1.00 20.00	6
	ATOM	1688	CB	ASN			65.403	14.137	5.930		
10	ATOM	1689	CG	ASN			64.342	13.825	-4.885	1.00 20.00	6
	ATOM	1690		ASN			64.292	14.450	-3.826	1.00 20.00	8
	ATOM	1691	ND2	ASN	В	286	63.477	12.861	-5.190	1.00 20.00	7
	MOTA	1692	C	ASN	В	286	67.076	15.042	-4.291	1.00 20.00	6
	ATOM	1693	0	ASN	В	286	67.368	14.682	-3.152	1.00 20.00	8
15	ATOM	1694	N	GLU	В	287	66.955	16.317	-4.636	1.00 20.00	٠7
10	ATOM	1695	CA	GLU			67.185	17.377	-3.669	1.00 20.00	6
				GLU			67.181	18.738	-4.365	1.00 20.00	6
	ATOM	1696	CB						-4.944	1.00 20.00	6
	ATOM	1697	CG	GLU			68.537	19.095			
	ATOM	1698	CD	GLU			68.524	20.385	-5.735	1.00 20.00	6
20	ATOM	1699		GLU			67.911	21.371	-5.267	1.00 20.00	8
	ATOM	1700	OE2	GLU	В	287	69.144	20.410	-6.823	1.00 20.00	8
	MOTA	1701	C	GLU	В	287	66.225	17.394	-2.492	1.00 20.00	6
	ATOM	1702	0	GLÜ	В	287	66.658	17.554	-1.354	1.00 20.00	8
	MOTA	1703	N	TYR	В	288	64.932	17.233	-2.753	1.00 20.00	7
25	ATOM	1704	CA	TYR			63.955	17.239	-1.670	1.00 20.00	6
23	ATOM	1705	CB	TYR			62.553	16.899	-2.184	1.00 20.00	6
			CG	TYR			61.530	16.780	-1.070	1.00 20.00	6
	ATOM	1706					60.984	17.917	-0:470	1.00 20.00	6
	ATOM	1707		TYR						1.00 20.00	6
	ATOM	1708		TYR			60.090	17.814	0.600		
30	MOTA	1709	CD2	TYR			61.154	15.529	-0.573	1.00 20.00	6
	MOTA	1710	CE2	TYR	В	288	60.265	15.414	0.498	1.00 20.00	
	ATOM	1711	CZ	TYR	В	288	59.740	16.561	1.078	1.00 20.00	6
	MOTA	1712	ОН	TYR	В	288	58.884	16.454	2.149	1.00 20.00	8.
	ATOM	1713	С	TYR	В	288	64.337	16.238	-0.587	1.00 20.00	6
35	ATOM	1714	Ó	TYR			64.254	16.545	0.598	1.00 20.00	8
33	ATOM	1715	N	LEU			64.750	15.041	-1.001	1.00 20.00	7
		1716	CA	LEU			65.137	13.989	-0.064	1.00 20.00	6
	ATOM			LEU			65.283	12.649	-0.797	1.00 20.00	6
	ATOM	1717	CB					11.985	-1.274	1.00 20.00	6
	MOTA	1718	CG	LEU			63.984			1.00 20.00	6.
40	ATOM	1719		LEU			64.314	10.802	-2.179		
	ATOM	1720	CD2	LEU			63.160	11.530	-0.068	1.00 20.00	6
	MOTA	1721	C	LEU			66.431	14.310	0.685	1.00 20.00	6
	MOTA	1722	0	LEU	В	289	66.604	13.914	1.840	1.00 20.00	8
	ATOM	1723	N			290	67.340	15.017	0.025	1.00 20.00	7
45	MOTA	1724,	CA	ILE	В	290	68.597	15.390	0.658	1.00 20.00	6
	ATOM	1725	CB	ILE			69.583	15.985	-0.366	1.00 20.00	6
	ATOM	1726		ILE			70.778	16.609	0.359	1.00 20.00	6
				ILE				14.887	-1.330	1.00 20.00	6
	ATOM	1727		ILE			70.844	15.398	-2.518	1.00 20.00	6
	MOTA	1728	_						1.743	1.00 20.00	
50	MOTA	1729	C,			290	68.307	16.424		1.00 20.00	
	MOTA	1730	0			290	68.807	16.317	2.862		
	MOTA	1731	N			291	67.491	17.420	1.411	1.00 20.00	
	MOTA	1732	CA	PHE	В	291	67.143	18.462	2.372	1.00 20.00	
	ATOM	1733	CB	PHE	В	291	66.222	19.502	1.731	1.00 20.00	
55	ATOM	1734	CG	PHE	В	291	66.869	20.289	0.628	1.00 20.00	
- •	ATOM	1735		PHE			68.255	20.420	0.568	1.00 20.00	6.
	ATOM	1736		PHE			66.094	20.931	-0.332	1.00 20.00	
	MOTA	1737		PHE			68.859	21.182	-0.435	1.00 20.00	6
				PHE			66.690	21.697	-1.340	1.00 20.00	
	ATOM	1738	CEZ	FILE	ם	4 J L	90.030	22.00,	_,_,		

	MOTA	1739	CZ	PHE	В	291	68.074	21.822	-1.390	1.00 20.00	6
	ATOM	1740	С	PHE	В	291	66.453	17.848	3.576	1.00 20.00	6
	ATOM	1741	0	PHE	В	291	66.664	18.262	4.718	1.00 20.00	8
	MOTA	1742	N	GLN			65.629	16.847	3.303	1.00 20.00	7
5	ATOM	1743	CA	GLN			64.887	16.154	4.341	1.00 20.00	6
-	ATOM	1744	CB	GLN			64.006	15.090	3.687	1.00 20.00	6
	ATOM	1745	CG	GLN			62.953	14.486	4.572	1.00 20.00	6
	ATOM	1746	CD	GLN			61.895	13.750	3.763	1.00 20.00	6
	ATOM	1747		GLN			62.208	12.835	2.997	1.00 20.00	8
10	ATOM	1748	NE2	GLN			60.637	14.155	3.924	1.00 20.00	7
10	ATOM	1749	C	GLN			65.865		5.329	1.00 20.00	
		1750	0	GLN				15.522			6
	ATOM		Ŋ	LYS			65.689	15.630	6.540	1.00 20.00	8
	ATOM	1751					66.907	14.875	4.812	1.00 20.00	7
1.5	ATOM	1752	CA	LYS			67.898	14.244	5.683	1.00 20.00	6
15	ATOM	1753	CB	LYS			68.850	13.372		1.00 20.00	6
	ATOM	1754	CG	LYS			68.197	12.135	4.278	1.00 20.00	6
	MOTA	1755	CD	LYS			69.217	11.260	3.554	1.00 20.00	6
	MOTA	1756	CE	LYS			68.575	9.972	3.051	1.00 20.00	6
	MOTA	1757	NZ	LYS			69.553	9.099	2.339	1.00 20.00	7
20	MOTA	1758	C	LYS			68.698	15.287	6.468	1.00 20.00	6
	MOTA	1759	0	LYS			69.044	15.074	7.634	1.00 20.00	8
	MOTA	1760	N	ILE	В	294	68.989	16.411	5.827	1.00 20.00	7
	MOTA	1761	CA	ILE	В	294	69.745	17.480	6.472	1.00 20.00	6
	MOTA	1762	CB	ILE	В	294	70.026	18.632	5.474	1.00 20.00	6
25	MOTA	1763	CG2	ILE	В	294	70.489	19.881	6.223	1.00 20.00	6
	ATOM	1764	CG1	ILE	В	294	71.070	18.178	4.443	1.00 20.00	6
	ATOM	1765	CD1	ILE	В	294	71.266	19.159	3.303	1.00 20.00	6
	MOTA	1766	С	ILE	В	294	69.035	18.045	7.712	1.00 20.00	6
	MOTA	1767	0	ILE	В	294	69.618	18.091	8.798	1.00 20.00	8
30	MOTA	1768	N	ILE	В	295	67.783	18.467	7.564	1.00 20.00	7
	ATOM	1769	CA	ILE	В	295	67.068	19.037	8.707	1.00 20.00	6
	ATOM	1770	CB	ILE	В	295	65.710	19.647	8.300	1.00 20.00	6
	ATOM	1771	CG2	ILE	В	295	65.927	20.749	7.265	1.00 20.00	6
	ATOM	1772	CG1	ILE			64.784	18.559	7.762	1.00 20.00	6
35	MOTA	1773	CD1	ILE			63.356	19.037	7.558	1.00 20.00	6
	MOTA	1774	C			295	66.831	18.045	9.842	1.00 20.00	6
	ATOM	1775	ō			295	66.540	18.447	10.967	1.00 20.00	8
	ATOM	1776	N	LYS			66.956	16.753	9.550	1.00 20.00	7
	ATOM	1777	CA	LYS			66.765	15.724	10.569	1.00 20.00	6
40	ATOM	1778	CB	LYS			65.907	14.576	10.019	1.00 20.00	6
	ATOM	1779	CG	LYS			64.535	15.010	9.538	1.00 20.00	6
	ATOM	1780	CD	LYS			63.739	13.851	8.951	1.00 20.00	6
	ATOM	1781	CE	LYS			63.296	12.873	10.025	1.00 20.00	· 6
	ATOM	1782	NZ	LYS			62.375	11.828	9.482	1.00 20.00	7
45					_		68.116	15.176		1.00 20.00	6
43	ATOM	1783	0	LYS			68.178	14.261	11.018	1.00 20.00	8
	ATOM	1784		LEU				15.746	10.474	1.00 20.00	7
. •	ATOM	1785	N	LEU			69.190	15.740			6
	ATOM	1786	CA				70.551		10.791	1.00 20.00	6
60	ATOM	1787	CB	LEU			70.911	15.680	12.236	1.00 20.00	
50	ATOM	1788	CG	LEU			72.398	15.538	12.585	1.00 20.00	6
	MOTA	1789		LEU			73.215	16.555		1.00 20.00	6
	ATOM	1790		LEU			72.605	15.762	14.076	1.00 20.00	6
	ATOM	1791	C	LEU			70.635	13.810	10.592	1.00 20.00	6
	ATOM	1792	0	LEU			71.150	13.080	11.434	1.00 20.00	8
55	ATOM	1793	N	GLU			70.128	13.351	9.456	1.00 20.00	7
	MOTA	1794	CA	GLU			70.115	11.934	9.148	1.00 20.00	6
	MOTA	1795	CB	GLU			68.817	11.597	8.416	1.00 20.00	6
	ATOM	1796	CG	GLU			68.568	10.123	8.233	1.00 20.00	6
	MOTA	1797	CD	GLU	В	298	67.254	9.858	7.535	1.00 20.00	6

	ATOM	1798	OE1	GLU	В	298		66.214	10.331	8.043	1.00 20.00	8
	MOTA	1799	OE2	GLU	В	298		67.261	9.185	6.484	1.00 20.00	8
	ATOM	1800	C	GLU	В	298		71.309	11.446	8.332	1.00 20.00	6
	MOTA	1801	0	GLU	В	298		71.310	11.523	7.104	1.00 20.00	8
5	ATOM	1802	N	TYR	В	299		72.325	10.946	9.027	1.00 20.00	7
_	ATOM	1803	CA	TYR	В	299		73.519	10.405	8.390	1.00 20.00	6
	ATOM	1804	CB	TYR				74.444	11.521	7.880	1.00 20.00	6
	ATOM	1805	CG	TYR				75.330	12.130	8.953	1.00 20.00	6
	ATOM	1806		TYR				74.796	12.962	9.935	1.00 20.00	6
10	ATOM	1807		TYR				75.589	13.482	10.951	1.00 20.00	6
10	MOTA	1808		TYR				76.692	11.833	9.013	1.00 20.00	6
	ATOM	1809		TYR				77.499	12.352	10.032	1.00 20.00	6
	ATOM	1810	CZ	TYR			•	76.935	13.173	10.032	1.00 20.00	6
	ATOM	1811	OH	TYR				77.701	13.687	12.006	1.00 20.00	8
15		1812	C	TYR				74.245	9.600		1.00 20.00	6
13	ATOM	.1813	0	TYR				73.913	9.688	10.631	1.00 20.00	8
	ATOM			ASP					8.808	9.052	1.00 20.00	7
	ATOM	1814	N					75.229		10.016	1.00 20.00	6
	ATOM	1815	CA	ASP				75.991	8.030	10.016	1.00 20.00	6
20	ATOM	1816	CB	ASP			•	75.291	6.700		1.00 20.00	6
20	MOTA	1817	.CG	ASP				74.898	5.968	9.048	1.00 20.00	8
	ATOM	1818		ASP				75.806	5.594	8.274	1.00 20.00	8
	ATOM	1819		ASP				73.681	5.771	8.832	1.00 20.00	6
	ATOM	1820	C	ASP				77.397	7.799	9.488		
0.5	ATOM	1821	0	ASP				77.651	7.976	8.297 10.378	1.00 20.00	7
25	MOTA	1822	N	PHE				78.307	7.417		1.00 20.00	6
	MOTA	1823	CA	PHE				79.695	7.186	9.996	1.00 20.00	6
	ATOM	1824	CB	PHE				80.655	7.664	11.093	1.00 20.00	6
	ATOM	1825	CG	PHE				80.488	9.103	11.481 12.370	1.00 20.00	6
20	ATOM	1826		PHE				79.493	9.487		1.00 20.00	6
30	ATOM	1827		PHE				81.346	10.075	10.970	1.00 20.00	6
	MOTA	1828				301		79.352	10.823 11.408	12.750 11.342	1.00 20.00	6
	MOTA	1829		PHE				81.214 80.215	11.783	12.235	1.00 20.00	6
	ATOM	1830	CZ			301			5.722	9.744	1.00 20.00	6
25	MOTA	1831	C			301		80.009 79.506	4.839	10.442	1.00 20.00	8
35	MOTA	1832	0			301			5.440	8.732	1.00 20.00	7
	MOTA	1833	И			302		80.842 81.330	6.316	7.654	1.00 20.00	6
	MOTA	1834	CD			302 302		81.191	4.044	8.466	1.00 20.00	6
	ATOM	1835	CA					81.838	4.105	7.084	1.00 20.00	6
40	MOTA	1836 1837	CB			302 302	•	82.425	5.479	7.046	1.00 20.00	6
40	MOTA	1838	CG C			302		82.168	3.629	9.569		6
	ATOM ATOM	1839	0			302		82.887	4.469	10.111	1.00 20.00	8
	ATOM	1840	N.			302		82.185	2.345	9.908	1.00 20.00	7
	ATOM	1841	CA			303		83.052	1.836	10.968	1.00 20.00	6
45		1842	CB	ALA				82.993	0.310		1.00 20.00	
43	ATOM ATOM	1843		ALA				84.513	2.294		1.00 20.00	6
	ATOM	1844	0	ALA				85.078	2.637	11.979	1.00 20.00	8
	ATOM	1845	И	ALA				85.121	2.306	9.756	1.00 20.00	7
	ATOM	1846	CA	ALA				86.527	2.684	9.605	1.00 20.00	6
50	ATOM	1847	CB			304		86.971	2.423	8.165	1.00 20.00	6
50	ATOM	1848	C			304		86.894	4.119	10.001	1.00 20.00	6
		1849	o			304		87.983	4.367	10.520	1.00 20.00	8
	ATOM ATOM	1850	N			304		85.985	5.053	9.742	1.00 20.00	7
	ATOM	.1851	CA			305		86.183	6.473	10.034	1.00 20.00	6
55	ATOM	1852	CB			305		84.822	7.115	10.312	1.00 20.00	
,,	ATOM	1853	CG			305		84.705	8.522	9.815	1.00 20.00	
	MOTA	1854		PHE				85.303	9.572	10.502	1.00 20.00	6
	ATOM	1855		PHE				84.003	8.800	8.646	1.00 20.00	
	ATOM	1856		PHE				85.202	10.881	10.033	1.00 20.00	

	ATOM	1857	CE2	PHE	B 3	05	83.896	10.106	8.167	1.00	20.00	6
	MOTA	1858	cz	PHE	B 3	05	84.496	11.147	8.862	1.00	20.00	6
	MOTA	1859	C	PHE	В 3	05	87.153	6.789	11.182	1.00	20.00	6
	ATOM	1860	0	PHE	В 3	05	86.964	6.342	12.312		20.00	8
5	ATOM	1861	N	PHE	B 3	06	88.190	7.565	10.883		20.00	7
	ATOM	1862	CA	PHE			89.176	7.945	11.894		20.00	6
	ATOM	1863	СВ	PHE			90.179	8.936	11.295		20.00	6
	ATOM	1864	CG	PHE			90.695	8.531	9.940		20.00	6
	ATOM	1865		PHE			91.292	7.284	9.747		20.00	6
10	ATOM	1866		PHE			90.588	9.395	8.853		20.00	6
	ATOM	1867		PHE	_		91.774	6.906	8.490		20.00	
	ATOM	1868	CE2	PHE	-			9.027				6
	ATOM	1869	CZ	PHE			91.067		7.590		20.00	6
		1870	C	PHE			91.662	7.780	7.408		20.00	6
15	ATOM						88.445	8.575	13.086		20.00	6
13	ATOM	1871	0	PHE			87.731	9.566	12.936		20.00	8
	ATOM	1872	N	PRO			88.614	7.995	14.288		20.00	7
	ATOM	1873	CD	PRO			89.482	6.834	14.555		20.00	6
	ATOM	1874	CA	PRO			87.983	8.459	15.530		20.00	6
	ATOM	1875	CB	PRO			88.748	7.691	16.606		20.00	6
20	ATOM	1876	CG	PRO :			89.018	6.388	15.928	1.00	20.00	6
	ATOM	1877	C	PRO	_		87.986	9.965	15.784		20.00	6
	ATOM	1878	0	PRO	B 3	07	86.936	10.565	16.025	1.00	20.00	8
	ATOM	1879	N	LYS :	B 3	80	89.162	10.575	15.745	1.00	20.00	7
	ATOM	1880	CA	LYS :	B 3	08	89.260	12.004	15.992	1.00	20.00	6
25	MOTA	1881	CB	LYS :	B 3	80	90.728	12.405	16.149	1.00	20.00	6
	MOTA	1882	CG	LYS	B 3	08	91.338	11.805	17.410	1.00	20.00	6
	MOTA	1883	$^{\mathtt{CD}}$	LYS :	B 3	08	92.806	12.140	17.591	1.00	20.00	6
	ATOM	1884	CE	LYS :	B 3	08	93.339	11.457	18.847	1.00	20.00	. 6
	ATOM	1885	NZ	LYS :	B 3	08 .	94.816	11.573	18.985	1.00	20.00	7
30	ATOM	1886	С	LYS :	В 3	08	88.572	12.808	14.894	1.00	20.00	6
	ATOM	1887	0	LYS :	В 30	08	87.985	13.855	15.167	1.00	20.00	8
	ATOM	1888	N	ALA :	B 3(09	88.629	12.318	13.659	1.00	20.00	7
	ATOM	1889	CA	ALA :	B 30	09	87.967	13.011	12.557	1.00	20.00	6
	ATOM	1890	CB	ALA :	B 3	09	88.328	12.369	11.231	1.00	20.00	6
35	ATOM	1891		ALA :			86.460	12.936	12.787		20.00	6
_	ATOM	1892	Ō	ALA			85.735	13.903	12.552		20.00	8
	ATOM	1893	N	ARG			85.986	11.780	13.246		20.00	7
	ATOM	1894	CA	ARG			84.561	11.619	13.513		20.00	6
	ATOM	1895	СВ	ARG			84.246	10.194	13.979		20.00	6
40	ATOM	1896	CG	ARG			82.844	10.069	14.561		20.00	6
	MOTA	1897	CD	ARG			82.408	8.632	14.789		20.00	6
	ATOM	1898	NE	ARG :			81.060	8.593	15.355		20.00	7.
	ATOM -	1899	CZ	ARG :			80.259	7.532	15.328		20.00	. 6
	ATOM	1900		ARG :			80.665	6.401	14.759		20.00	7
45	ATOM	1901		ARG :			79.048	7.601	15.867		20.00	7
43	ATOM	1902					84.110	12.613			20.00	6
	ATOM	1902	C	ARG :				13.274	14.583			
			0	ARG :			83.080		14.436		20.00	8
	ATOM	1904	N	ASP :			84.876	12.707	15.666		20.00	7
	ATOM	1905	CA	ASP :			84.535	13.629	16.740		20.00	6
50	MOTA	1906	CB	ASP :			85.574	13.555	17.864		20.00	6
	ATOM	1907		ASP :			85.260	14.505	19.006		20.00	6
	MOTA	1908		ASP :			85.782	15.636	19.010		20.00	8
	MOTA	1909		ASP :			84.480	14.124	19.901		20.00	8
	MOTA	1910	С	ASP :			84.445	15.054	16.198		20.00	6
55	MOTA	1911	0	ASP :			83.539	15.800	16.564		20.00	8
	ATOM	1912	N	LEU :			85.371	15.423	15.313		20.00	7
	MOTA	1913	CA	LEU :			85.362	16.769	14.736		20.00	6
	MOTA	1914	CB	LEU :			86.604	16.999	13.869		20.00	6
	MOTA	1915	CG	LEU :	B 3:	12	86.662	18.329	13.099	1.00	20.00	6

													,		
	ATOM	1916	CD1	LEU 1	3 31	2	86	.424	19.	510	14.0	37	1.00	20.00	6
	ATOM	1917	CD2	PER 1	3 31	2	88	.018	18.	450	12.4			20.00	6
	ATOM	1918	C	PEA 1	3 31	2	84	.112	17.	800	13.8	199		20.00	6
	ATOM	1919	0	LEU 1	3 3 1	2	83	.456	18.		14.0			20.00	8
5	MOTA	1920	N	VAL 1	3 3 1	3	83	.786	16.	051	13.0			20.00	7
	MOTA	1921	CA	VAL 1	3 3 1	3	82	.611	16.	171	12.1			20.00	6
	ATOM	1922	CB	VAL 1	3 3 1	3	82	.464	14.		11.2			20.00	6
	ATOM	1923		VAL I		3	81	.121	14.		10.5			20.00	6
	ATOM	1924		VAL 1	B 31	3		. 595	14.		10.2			20.00	6
10	ATOM	1925	C	VAL				.354	16.		13.0			20.00	6
	MOTA	1926	0	VAL :				.467	17.		12.7			20.00	8
	ATOM	1927	И	GLU :				.282	15.		14.1			20.00	7
	ATOM	1928	CA	GLU :				.122	15.		15.0			20.00	6
	ATOM ·	1929	CB	GLU :				.191	14.		16.0			20.00	6
15	MOTA	1930	CG	GLU :				.160	13.		15.5			20.00	6
	MOTA	1931	CD	GLU				.222	12.		16.6			20.00	6
	ATOM	1932	OE1					.033	12.		17.			20.00	8
	MOTA	1933	OE2	GLU				.469		081	16.5			20.00	8
	MOTA	1934	С	GLU				.035	17.		15.6			20.00	6
20	MOTA	1935	0	GLU				.960		443	16.0			20.00	8 7
	MOTA	1936	N	LYS				.165		690	15.			20.00	6
	ATOM	1937	CA	LYS				.154		010	16.			20.00	6
	MOTA	1938	CB	LYS				.448		240	17.			20.00	6
	ATOM	1939	CG	LYS				.460		478	18.4 19.3			20.00	6
25	MOTA	1940	CD	LYS				.803		529	20.			20.00	6
	ATOM	1941	CE	LYS				.749		825 505	21.			20.00	7
	ATOM	1942	NZ	LYS				.829		104	15.			20.00	6
	ATOM	1943	C	LYS				.934 .855		282	15.			20.00	8
20	MOTA	1944	0	LYS				.819		706	14.			20.00	7
30	ATOM	1945	N	LEU LEU				.577		649	12.			20.00	6
	MOTA	1946	CA	LEU				.608		450	11.			20.00	6
	MOTA	1947	CB CG	LEU				.044		833	12.			20.00	6
	ATOM	1948		LEU				.011		365	11.			20.00	6
25	ATOM	1949 1950		LEU				.124		351	12.			20.00	6
35	ATOM ATOM	1951	CDZ	LEU				.164		469	12.		1.00	20.00	6
	ATOM	1952	Ö	LEU				.464		448	12.		1.00	20.00	8
	ATOM	1953	N	LEU				.746		.220	12.	230 ^c	1.00	20.00	• 7
	ATOM	1954	CA	LEU				.403		962	11.	721	1.00	20.00	6
40	ATOM	1955	CB	LEU				.343	17.	. 605	11.	012		20.00	
	ATOM	1956	CG	LEU			78	3.335	17	.445	9.	852	1.00	20.00	6
	ATOM	1957		LEU			78	3.091	16	.111	9.	143	1.00	20.00	6
	ATOM	1958	CD2	LEU	B 3	17	78	3.182	18.	.603	8.	866	1.00	20.00	
	ATOM	1959	С	LEU	В 3	17	76	5.435	19	.000		899		20.00	
45	ATOM	1960	0	LEU	B 3	17	75	5.979	17	. 966	13.	398		20.00	
	ATOM	1961	N	VAL	B 3	18	76	5.156	20	215	13.	354		20.00	
	ATOM	1962	CA	VAL			75	5.251	20	.451	14.	467		20.00	
	ATOM	1963	CB	VAL	B 3	18	75	5.981	21	.164	15.	625		20.00	
	MOTA	1964	CG1	VAL	B 3	18	75	5.007		.461		759		20.00	
50	MOTA	1965	CG2	VAL	B 3	18		7.136		.300		115		20.00	
	MOTA	1966	С	VAL				1.140				936		20.00	
	MOTA	1967	0	VAL				4.410		.386		333		20.00	
	MOTA	1968	N	LEU				2.892		.941		153		20.00	
	ATOM	1969	CA	LEU				1.758		.717		663		20.00	
55	ATOM	1970	CB		B 3			0.444		.056		093		20.00	
	MOTA	1971	. CG		B 3			0.211		.647		533		20.00	
	MOTA	1972		LEU				8.883		.098		060		0 20.00	
	ATOM	1973		LEU.				0.211		.688		000		0 20.00	
	ATOM	1974	С	LEU	в 3	19	7	1.794	23	.173	14.	.119	1.0	0 20.00	, 0

	MOTA	1975	0	LEU	В	319		71.591	24.082	13.317	1.00		8
	ATOM	1976	N	ASP				72.052	23.394	15.405	1.00 2		7
	MOTA	1977	CA	ASP	В	320		72.119	24.745	15.958	1.00	20.00	6
	ATOM	1978	CB	ASP	В	320		72.091	24.687	17.490	1.00 2	20.00	6
5	ATOM	1979	CG	ASP	В	320		72.058	26.061	18.129	1.00 2	20.00	6
	ATOM	1980	OD1	ASP	В	320		72.506	27.036	17.492	1.00	20.00	8
	ATOM	1981	OD2	ASP	В	320		71.595	26.166	19.284	1.00	20.00	8
	ATOM	1982	С	ASP	В	320		73.415	25,419	15.492	1.00	20.00	6
	ATOM	1983	0	ASP	В	320		74.496	25.089	15.965	1.00	20.00	8
10	MOTA	1984	N·	ALA	В	321		73.294	26.372	14.576	1.00	20.00	7
	ATOM	1985	CA	ALA	В	321		74.450	27.078	14.028	1.00	20.00	6′
	ATOM	1986	CB	ALA				73.982	28.109	13.006	1.00	20.00	6
	ATOM	1987	C	ALA				75.359	27.747	15.065	1.00	20.00	6
	ATOM	1988	0	ALA				76.535	27.992	14.790	1.00	20.00	8
15	ATOM	1989	Ŋ	THR				74.829	28.035	16.252	1.00	20.00	7
	ATOM	1990	CA	THR				75.631	28.681	17.292	1.00	20.00	6
	ATOM	1991	CB	THR				74.755	29.491	18.271	1.00	20.00	6
	ATOM	1992		THR				73.879	28.605	18.973	1.00		8
	ATOM	1993	CG2	THR				73.928	30.527	17.519	1.00		6
20	ATOM	1994	C	THR				76.437	27.684	18.108	1.00		6
20	ATOM	1995	ō	THR				77.166	28.071	19.019	1.00	20.00	8
	ATOM	1996	N	LYS				76.312	26.401	17.786	1.00		7
	ATOM	1997	CA	LYS				77.048	25.378	18.517	1.00		6
		1998	CB	LYS				76.080	24.378	19.155	1.00		6
25	MOTA	1999	CG	LYS				75.180	24.992	20.209	1.00		6
23	ATOM	2000	CD	LYS				74.356	23.931	20.924	1.00		6
	ATOM		CE	LYS				73.406	24.574	21.927	1.00		6
	MOTA	2001 2002	NZ	LYS				74.144	25.514	22.818	1.00		7
	ATOM	2002	C	LYS				78.066	24.631	17.664	1.00		6
20	ATOM		0	LYS				78.520	23.557	18.040	1.00		8
30	ATOM	2004	N	ARG				78.427	25.195	16.517	1.00		7
	ATOM	2005	CA	ARG				79.408	24.545	15.656		20.00	6
	ATOM	2006	CB	ARG				79.108	24.834	14.186		20.00	6
	ATOM	2007	CG			324		77.824	24.177	13.728		20.00	6
25	MOTA	2008	CD			324		77.468	24.505	12.297		20.00	6
35	MOTA	2009	NE			324		76.060	24.202	12.069		20.00	7
	ATOM	2010 2011	CZ			324		75.277	24.873	11.233		20.00	6
,	MOTA	2011		ARG				75.764	25.888	10.523		20.00	7
	ATOM	2012		ARG				73.992	24.551	11.140		20.00	7
40	MOTA	2013	C			324		80.811	25.011	16.008		20.00	6
40	ATOM ATOM	2014	0			324		81.070	26.212	16.131		20.00	8
	ATOM	2015	N	LEU		325		81.711	24.049	16.180		20.00	7
	ATOM	2010	CA			325		83.090	24.350	16.520		20.00	6
		2017	CB			325		83.913	23.061	16.550		20.00	6
45	ATOM	2018	CG			325		85.274	23.123	17.241		20.00	6
43	MOTA			LEU				85.093	23.591	18.682		20.00	6
	MOTA	2020		LEU				85.922	21.741	17.209		20.00	6
	MOTA	2021				325		83.656	25.310	15.481		20.00	6
	ATOM	2022	C			325		83.649	25.015	14.282		20.00	8
c 0	ATOM	2023	0			326		84.139	26.461	15.946		20.00	7
50	ATOM	2024	N			326 ⁻		84.697	27.449	15.040		20.00	6
	MOTA	2025	CA			326		83.857	28.711	14.932		20.00	6
	ATOM	2026	C			326	•	84.369	29.757	14.529		20.00	8
	MOTA	2027	O N					82.575	28.632	15.286		20.00	7
	ATOM	2028	N			327			29.806	15.200		20.00	6
55	MOTA	2029	CA			327 327		81.714 80.233	29.404	15.183		20.00	6
	MOTA	2030	CB			327		79.534		16.774		20.00	
	ATOM	2031	SG			327		81.976	30.772	16.353		20.00	6
	ATOM	2032	C			327		82.565	30.772	17.371		20.00	8
	MOTA	2033	0	CIS	ם	241		02.303	30.410	,,,,,,,		•	

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	MOTA	2034	N	GLU	В	328	81.523	32.005	16.178	1.00 20.00	7
	ATOM	2035	CA	GLU	В	328	81.714	33.052	17.167	1.00 20.00	6
	ATOM	2036	СВ	GLU			81.087	34.348	16.632	1.00 20.00	
	ATOM	2037	CG	GLU			81.734	34.772	15.300	1.00 20.00	
5	ATOM	2038	CD	GLU			80.962	35.842	14.539	1.00 20.00	
•	ATOM	2039		GLU			79.738	35.676	14.343	1.00 20.00	
	ATOM	2040	OE2	GLU			81.588	36.840	14.116	1.00 20.00	
	ATOM	2041	C	GLU			81.187	32.701	18.560	1.00 20.00	
	ATOM	2012	ō	GLU			81.850	32.983	19.562	1.00 20.00	
10	ATOM	2043	N	GLU			80.016	32.073	18.631	1.00 20.00	
10	MOTA	2044	CA	GLU			79.449	31.714	19.926	1.00 20.00	
	ATOM	2045	CB	GLU			77.991	31.714	19.782	1.00 20.00	
	ATOM	2045	CG	GLU			77.028	32.355	19.315	1.00 20.00	
	ATOM	2047	CD	GLU			77.025	32.575	17.813	1.00 20.00	
15	ATOM	2047		GLU			77.859	31.910	17.120	1.00 20.00	
13		2048	OE2	GLU				33.413	17.323	1.00 20.00	
	ATOM		C	GLU			76.267			1.00 20.00	
	ATOM	2050	0				80.264	30.616	20.605	1.00 20.00	
	ATOM	2051		GLU MET			80.182	30.436	21.819	1.00 20.00	
20	ATOM	2052	N				81.040	29.878	19.816	1.00 20.00	
20	ATOM	2053	CA	MET			81.880	28.813	20.354		
	ATOM	2054	CB	MET			81.872	27.600	19.419	1.00 20.00	
	ATOM	2055	CG	MET			80.552	26.822	19.436	1.00 20.00	
	MOTA	2056	SD	MET			80.117	26.254	21.104	1.00 20.00	
25	ATOM	2057	CE	MET			81.265	24.895	21.311	1.00 20.00	
25	ATOM	2058	C	MET			83.302	29.330	20.547	1.00 20.00	
	ATOM	2059	0	MET			84.236	28.564	20.754	1.00 20.00	
	ATOM	2060	N	GLU			83.443	30.647	20.471	1.00 20.00	
	ATOM	2061	CA	GLU			84.716	31.338	20.656	1.00 20.00	
20	ATOM	2062	CB	GLU			85.357	30.921	21.987	1.00 20.00	
30	MOTA	2063	CG	GLU			84.371	30.886	23.163	1.00 20.00	
	MOTA	2064	CD	GLU			83.478	32.127	23.270	1.00 20.00	
	ATOM	2065	OE1	GLU			82.483	32.064	24.021	1.00 20.00	
	ATOM	2066	OE2	GLU				33.159	22.625	1.00 20.00	
2.5	ATOM	2067	C	GLU			85.742	31.247	19.523	1.00 20.00	
35	ATOM	2068	0			331	86.952	31.264	19.761	1.00 20.00	
	MOTA	2069	N	GLY			85.257	31.137	18.292	1.00 20.00	
	ATOM	2070	CA	GLY			86.145	31.159	17.140	1.00 20.00	
	ATOM	2071	C	GLY			87.036	30.014	16.721	1.00 20.00	
40	MOTA	2072	0	GLY			86.881	28.863	17.142	1.00 20.00	
40	MOTA	2073	N	TYR			88.002	30.366	15.875	1.00 20.00	
	MOTA	2074	CA	TYR			88.939	29.413	15.307	1.00 20.00	
	ATOM	2075	CB	TYR			89.625	30.053	14.093	1.00 20.00	
	MOTA	2076	CG	TYR			88.724	30.031	12.877	1.00 20.00	
	ATOM	2077		TYR				28.966	11.974	1.00 20.00	
45	MOTA	2078		TYR			87.872	28.869	10.919	1.00 20.00	
	MOTA	2079		TYR			87.747	31.011	12.686	1.00 20.00	
•	ATOM	2080		TYR			86.831	30.923	11.624	1.00 20.00	
•	ATOM	2081	CZ	TYR			86.903	29.845	10.751	1.00 20.00	
	ATOM	2082	OH	TYR			86.001	29.719	9.724	1.00 20.00	
50	MOTA	2083	С	TYR			89.958	28.800	16.252	1.00 20.00	
	MOTA	2084	0	TYR			90.473	27.721	15.971	1.00 20.00	
	ATOM	2085	N	GLY			90.242	29.469	17.369	1.00 20.00	
	ATOM	2086	CA	GLY			91.193	28.921	18.327	1.00 20.00	
	MOTA	2087	C	GLY			90.803	27.504	18.741	1.00 20.00	
55	MOTA	2088	0	GLY			91.577	26.564	18.558	1.00 20.00	
	ATOM	2089	N	PRO			89.603	27.320	19.309	1.00 20.00	
	ATOM	2090	CD	PRO			88.703	28.372	19.814	1.00 20.00	
	ATOM	2091	CA	PRO			89.145	25.991	19.731	1.00 20.00	
	MOTA	2092	CB	PRO	ㅂ	335	87.759	26.275	20.303	1.00 20.00) 6

	ATOM	2093	CG	PRO	В	335	87.925	27.644	20.883	1.00 20.00	6
	ATOM	2094	С	PRO	В	335	89.104	24.986	18.573	1.00 20.00	6
	MOTA	2095	0	PRO	В	335	89.406	23.808	18.756	1.00 20.00	8
	ATOM	2096	N	LEU	В	336	88.727	25.450	17.382	1.00 20.00	7
5	MOTA	2097	CA	LEU	В	336	88.666	24.567	16.219	1.00 20.00	6
	ATOM	2098	·CB	LEU	В	336	88.031	25.292	15.023	1.00 20.00	6
	MOTA	2099	CG	LEU	В	336	88.051	24.581	13.663	1.00 20.00	6
	ATOM	2100	CD1	LEU	В	336	87.486	23.177	13.787	1.00 20.00	6
	ATOM	2101	CD2	LEU	В	336	87.239	25.399	12.653	1.00 20.00	6
10	ATOM	2102	С	LEU	В	336	90.060	24.068	15.839	1.00 20.00	6
	ATOM	2103	0	LEU	В	336	90.274	22.870	15.665	1.00 20.00	8
	ATOM	2104	И	LYS	В	337	91.011	24.986	15.717	1.00 20.00	7
	MOTA	2105	CA	LYS	В	337	92.370	24.597	15.360	1.00 20.00	6
	ATOM	2106	CB	LYS	В	337	93.198	25.848	15.046	1.00 20.00	٠6
15	ATOM	2107	CG	LYS		337	92.678	26.560	13.801	1.00 20.00	6
	MOTA	2108	CD	LYS	В	337	93.111	28.014	13.717	1.00 20.00	6
	ATOM	2109	CE	LYS	В	337	94.561	28.167	13.314	1.00 20.00	6
	MOTA	2110	NZ	LYS	В	337	94.882	29.611	13.122	1.00 20.00	7
	ATOM	2111	С	LYS	В	337	93.020	23.764	16.467	1.00 20.00	6
20	MOTA	2112	0	LYS		337	93.965	23.015	16.215	1.00 20.00	8
	ATOM	2113	N	ALA			92.495	23.866	17.684	1.00 20.00	7
	ATOM -		CA	ALA		338	93.056	23.105	18.799	1.00 20.00	6
	MOTA	2115	CB	ALA		338	92.873	23.877	20.105	1.00 20.00	6
	ATOM	2116	С	ALA		338	92.441	21.718	18.929	1.00 20.00	6
25 .	ATOM	2117	0	ALA		338	92.805	20.955	19.820	1.00 20.00	8
	ATOM	2118	N	HIS		339	91.513	21.375	18.043	1.00 20.00	7
	ATOM	2119	,CA	HIS			90.886	20.061	18.129	1.00 20.00	6
	ATOM	2120	CB	HIS		339	89.786	19.919	17.074	1.00 20.00	6
20	ATOM	2121	CG	HIS		339	88.999	18.654	17.199	1.00 20.00	6
30	ATOM	2122		HIS		339	87.797	18.406	17.774	1.00 20.00	6
	ATOM	2123		HIS		339	89.462	17.440	16.737	1.00 20.00	7
	MOTA	2124		HIS		339	88.578	16.498	17.021	1.00 20.00	6 7
	ATOM	2125		HIS		339	87.559	17.057	17.650 17.970	1.00 20.00	6
35	MOTA	2126 2127	С 0	HIS		339 339	91.928 92.863	18.952 19.077	17.186	1.00 20.00	8
33	ATOM ATOM	2127	N	PRO		340	91.780	17.854	18.731	1.00 20.00	7
	ATOM	2129	CD	PRO		340	90.747	17.655	19.765	1.00 20.00	6
	ATOM	2130	CA	PRO		340	92.700	16.711	18.694	1.00 20.00	6
	ATOM	2131	CB	PRO			91.966	15.665	19.521	1.00 20.00	6
40	ATOM	2132	CG	PRO		340	91.310	16.505	20.579	1.00 20.00	6
	ATOM	2132	C	PRO		340	93.072	16.198	17.301	1.00 20.00	6
	ATOM	2134	ō	PRO		340	94.193	15.748	17.080	1.00 20.00	8
	ATOM	2135	Ŋ	PHE		341	92.139	16.270	16.362	1.00 20.00	7
	ATOM	2136	CA	PHE			92.407	15.797	15.011	1.00 20.00	6
45	ATOM	2137	CB	PHE			91.152	15.943	14.142	1.00 20.00	6
	ATOM	2138	CG	PHE			91.317	15.424	12.738	1.00 20.00	6
	ATOM	2139		PHE			91.596	14.080	12.507	1.00 20.00	6
	ATOM	2140		PHE			91.182	16.277	11.647	1.00 20.00	6
	ATOM	2141		PHE			91.738	13.592	11.207	1.00 20.00	6
50	ATOM	2142		PHE			91.320	15.803	10.345	1.00 20.00	6
	ATOM	2143	CZ	PHE			91.599	14.457	10.123	1.00 20.00	6
	ATOM	2144	C	PHE	В	341	93.571	16.550	14.362	1.00 20.00	6
	MOTA	2145	0	PHE			94.268	16.002	13.514	1.00 20.00	8
	ATOM	2146	N	PHE	В	342	93.777	17.800	14.765	1.00 20.00	7
55	MOTA	2147	CA	PHE			94.842	18.630	14.202	1.00 20.00	6
	ATOM	2148	CB	PHE	В	342	94.336	20.058	13.975	1.00 20.00	6
	ATOM	2149	CG	PHE			93.124	20.152	13.096	1.00 20.00	6
	MOTA	2150		PHE			93.166	19.729	11.777	1.00 20.00	6
	ATOM	2151	CD2	PHE	В	342	91.954	20.734	13.575	1.00 20.00	6

	ATOM	2152	CE1	PHE	В	342	92.058	19.888	10.936	1.00 20.00	6
	MOTA	2153	CE2	PHE	В	342	90.843	20.898	12.742	1.00 20.00	6
	ATOM	2154	CZ	PHE	В	342	90.898	20.475	11.423	1.00 20.00	6
	MOTA	2155	С	PHE	В	342	96.077	18.718	15.101	1.00 20.00	6
5	ATOM	2156	0	PHE	В	342	96.932	19.584	14.902	1.00 20.00	8
	ATOM	2157	N	GLU	В	343	96.173	17.829	16.083	1.00 20.00	7
	ATOM	2158	CA	GLU			97.293	17.857	17.022	1.00 20.00	6
	ATOM	2159	CB	GLU			97.330	16.564	17.841	1.00 20.00	6
	ATOM	2160	CG	GLU			98.475	16.525	18.839	1.00 20.00	6
10	ATOM	2161	CD	GLU			98.372	15.365	19.813	1.00 20.00	6
10	ATOM	2162		GLU			98.290	14.201	19.359	1.00 20.00	8
	ATOM	2163		GLU			98.379	15.622	21.036	1.00 20.00	8
	ATOM	2164	C	GLU		-	98.683	18.113	16.430	1.00 20.00	6
	ATOM	2165	0	GLU			99.419	18.969	16.925	1.00 20.00	8
15		2166	N	SER			99.047	17.382	15.383	1.00 20.00	7
13	ATOM						100.370	17.549	14.781	1.00 20.00	6
	ATOM	2167	CA	SER					14.701	1.00 20.00	6
	MOTA	2168	CB	SER			100.848	16.219		1.00 20.00	8
	ATOM	2169	OG	SER			100.072	15.856	13.065		6
20	ATOM	2170	C	SER			100.467	18.629	13.702	1.00 20.00	
20	MOTA	2171	0	SER			101.485	18.732	13.025	1.00 20.00	8
	MOTA	2172	N	VAL			99.423	19.435	13.544	1.00 20.00	7
	MOTA	2173	CA	VAL			99.430	20.486	12.527	1.00 20.00	6
	MOTA	2174	CB	VAL			97.985	20.843	12.075	1.00 20.00	6
	MOTA	2175		VAL			98.015	22.042	11.120	1.00 20.00	6
25	MOTA	2176	CG2	VAL			97.335	19.646	11.400	1.00 20.00	6
	ATOM	2177	С	VAL			100.096	21.785	12.980	1.00 20.00	6
	MOTA	2178	0	VAL			99.844	22.275	14.085	1.00 20.00	8
	MOTA	2179	N	THR			100.951	22.335	12.122	1.00 20.00	7
	ATOM	2180	CA	THR		346	101.602	23.610	12.397	1.00 20.00	6
30	ATOM	2181	CB	THR	В	346	103.096	23.593	11.982	1.00 20.00	6
	MOTA	2182	OG1	THR		346	103.816	22.688	12.831	1.00 20.00	8
	MOTA	2183	CG2	THR	В	346	103.707	24.983	12.115	1.00 20.00	6
	MOTA	2184	С	THR	В	346	100.810	24.573	11.510	1.00 20.00	6
	MOTA	2185	0	THR	В	346	100.950	24.565	10.285	1.00 20.00	8
35	MOTA	2186	N	TRP	В	347	99.966	25.385	12.138	1.00 20.00	7
	MOTA	2187	CA	TRP	В	347	99.089	26.306	11.425	1.00 20.00	6
	MOTA	2188	CB	TRP	В	347	97.941	26.727	12.344	1.00 20.00	6
	ATOM	2189	CG	TRP	В	347	97.088	25.594	12.818	1.00 20.00	6
	MOTA	2190	CD2	TRP	В	347	95.924	25.071	12.165	1.00 20.00	6
40	ATOM	2191	CE2	TRP	В	347	95.436	24.008	12.963	1.00 20.00	6
	ATOM	2192	CE3	TRP	В	347	95.247	25.397	10.983	1.00 20.00	6
	ATOM	2193	CD1	TRP	В	347	97.259	24.848	13.953	1.00 20.00	6
	ATOM	2194	NE1	TRP	B	347	96.269	23.893	14.048	1.00 20.00	7
	ATOM	2195	CZ2	TRP	В	347	94.300	23.270	12.616	1.00 20.00	б
45	ATOM	2196	CZ3	TRP	В	347	94.113	24.661	10.636	1.00 20.00	6
	ATOM	2197		TRP			93.654	23.610	11.452	1.00 20.00	6
	ATOM	2198	С	TRP	В	347	99.679	27.563	10.800	1.00 20.00	6
	ATOM	2199	0			347	99.101	28.114	9.867	1.00 20.00	8
	ATOM	2200	N			348	100.820	28.016	11.308	1.00 20.00	7
50	ATOM	2201	CA			348	101.439	29.247	10.822	1.00 20.00	6
	ATOM	2202	CB			348	102.582	29.656	11.761	1.00 20.00	6
	ATOM	2203	С			348	101.933	29.277	9.381	1.00 20.00	6
	ATOM	2204	ō			348	101.874	30.323	8.738	1.00 20.00	8
	ATOM	2205	N			349	102.411	28.152	8.860	1.00 20.00	7
55	ATOM	2206	CA			349	102.940	28.153	7.500	1.00 20.00	6
J J	MOTA	2207	CB			349	104.466	28.205	7.569	1.00 20.00	6
	ATOM	2208	CG			349	105.058	26.929	8.138	1.00 20.00	6
	ATOM	2209		ASN			104.445	26.282	8.984	1.00 20.00	8
	ATOM	2210		ASN			106.251	26.563	7.678	1.00 20.00	7
	WION	2220	.,,,,,,,,,,								

	MOTA	2211	C	ASN I	B 349	102.522	26.966	6.634	1.00 20.00	6
	MOTA	2212	0	ASN 1	B 349	103.353	26.371	5.944	1.00 20.00	
	MOTA	2213	N	LEU I	B 350	101.242	26.628	6.643	1.00 20.00	7
	MOTA	2214	CA	LEU 1	350	100.776	25.500	5.846	1.00 20.00	6
5	ATOM	2215	CB	LEU I	350	99.257	25.355	5.973	1.00 20.00	6
	ATOM	2216	CG	LEU I	350	98.734	24.848	7.316	1.00 20.00	6
	ATOM	2217	CD1	LEU I		97.244	25.127	7.418	1.00 20.00	
	ATOM	2218		LEU I		99.030	23.357	7.444	1.00 20.00	6 6
	ATOM	2219	C	LEU I		101.147	25.574			
10	ATOM	2220	Ō	LEU I		101.557		4.365	1.00 20.00	6
	ATOM	2221	N	HIS E		101.006	24.575	3.775	1.00 20.00	8
	ATOM	2222	CA	HIS E		101.305	26.744	3.752	1.00 20.00	7
	ATOM	2223	CB	HIS E		100.651	26.829	2.329	1.00 20.00	6
	ATOM	2224	CG	HIS E			28.087	1.721	1.00 20.00	6
15	ATOM	2225		HIS E		101.553	29.274	1.618	1.00 20.00	6
13						102.001		2.556	1.00 20.00	6
	ATOM	2226		HIS E		102.072	29.706	0.416	1.00 20.00	7
	ATOM	2227		HIS E		102.798	30.792	0.618	1.00 20.00	6
	ATOM	2228	NE2			102.772	31.079	1.907	1.00 20.00	7
20	ATOM	2229	C	HIS E		102.797	26.731	1.999	1.00 20.00	6
20	ATOM	2230	0	HIS E		103.176	26.669	0.832	1.00 20.00	8
	ATOM	2231	N	GLN E		103.634	26.685	3.033	1.00 20.00	7
	ATOM	2232	CA	GLN E		105.081	26.554	2.851	1.00 20.00	6
	MOTA	2233	CB	GLN E		105.841	27.458	3.819	1.00 20.00	6
	ATOM	2234	CG	GLN E		106.395	28.705	3.166	1.00 20.00	6
25	ATOM	2235	CD	GLN E	352	105.930	29.966	3.854	1.00 20.00	6
	ATOM	2236	OE1	GLN E	352	106.134	30.139	5.053	1.00 20.00	8
	ATOM	2237	NE2	GLN B	352	105.299	30.854	3.096	1.00 20.00	7
	ATOM	2238	C	GLN B	352	105.478	25.099	3.088	1.00 20.00	6
	ATOM	2239	0	GLN B	352	106.632	24.715	2.895	1.00 20.00	8
30	MOTA	2240	N	GLN B	353	104.514	24.295	3.522	1.00 20.00	7
	ATOM	2241	CA	GLN B		104.761	22.888	3.777	1.00 20.00	6
	ATOM	2242	CB	GLN B	353	103.849	22.395	4.900	1.00 20.00	6
	ATOM	2243	CG	GLN B		104.122	23.050	6.240	1.00 20.00	6
	ATOM	2244	CD	GLN B		103.075	22.711	7.281	1.00 20.00	6
35	ATOM	2245	OE1	GLN B		102.627	21.571	7.377	1.00 20.00	8
	ATOM	2246	NE2			102.690	23.700	8.076	1.00 20.00	7
	ATOM.	2247	С	GLN B		104.507	22.079	2.510	1.00 20.00	6
	ATOM	2248	ō	GLN B		103.732	22.490	1.641	1.00 20.00	
	ATOM	2249	N	THR B		105.732	20.937		1.00 20.00	8
40	ATOM	2250	CA	THR B		104.998	20.071	2.401		7
	ATOM	2251	CB	THR B		104.330	19.173	1.244	1.00 20.00	6
	ATOM	2252		THR B		106.240		1.029	1.00 20.00	6
	ATOM	2253		THR B		106.033	19.999	0.790	1.00 20.00	8
	ATOM	2254	C	THR B		•	18.243	-0.166	1.00 20.00	6
45	ATOM	2255	0			103.777	19.197	1.501	1.00 20.00	6
-13	ATOM	2256	N	THR B		103.745	18.426	2.454	1.00 20.00	8
	ATOM	2257	CD	PRO B		102.741	19.319	0.658	1.00 20.00	7
				PRO B		102.547	20.275	-0.444	1.00 20.00	6
	ATOM	2258	CA	PRO B		101.540	18.505	0.859	1.00 20.00	6
50	ATOM	2259	CB	PRO B		100.616	18.967	-0.266	1.00 20.00	6
50	ATOM	2260	CG	PRO B		101.039	20.387	-0.490	1.00 20.00	6
	ATOM	2261	C	PRO B		101.835	17.011	0.766	1.00 20.00	6
•	ATOM	2262	0	PRO B		102.631	16.577	-0.065	1.00 20.00	8
	ATOM	2263	N	PRO B		101.198	16.204	1.625	1.00 20.00	7
	MOTA	2264	CD	PRO B		100.128	16.522	2.587	1.00 20.00	6
55	MOTA	2265	CA	PRO B		101.438	14.761	1.573	1.00 20.00	6
	MOTA	2266	CB	PRO B		100.593	14.235	2.729	1.00 20.00	6
	ATOM	2267	CG	PRO B		99.429	15.188	2.737	1.00 20.00	6
	MOTA	2268	С	PRO B		100.960	14.244	0.222	1.00 20.00	6
	MOTA	2269	0	PRO B	356	100.005	14.779	-0.346	1.00 20.00	8

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	ATOM	2270	N	ALA	В	357		101.629	13.221	-0.300	1.00 20.00	7	
	ATOM	2271	CA	ALA	В	357		101.247	12.660	-1.588	1.00 20.00	6	
	MOTA	2272	CB	ALA	В	357		102.352	11.750	-2.118	1.00 20.00	6	
	ATOM	2273	C	ALA	В	357		99.948	11.883	-1.427	1.00 20.00	6	
5	ATOM	2274	0	ALA	В	357		99.808	11.074	-0.506	1.00 20.00	8	
	MOTA	2275	N	LEU	В	358		99.000	12.134	-2.323	1.00 20.00	7	`
	ATOM	2276	CA	LEU				97.709	11.460	-2.278	1.00 20.00	6	
	MOTA	2277	СВ	LEU				96.729	12.166	-3.217	1.00 20.00	6	
	ATOM	2278	CG	LEU				96.368	13.582	-2.766	1.00 20.00	6	
10	MOTA	2279		LEU				95.513	14.262	-3.813	1.00 20.00	6	•
••	ATOM	2280		LEU				95.636	13.516	-1.430	1.00 20.00	6	
	MOTA	2281	C	LEU				97.813	9.976	-2.633	1.00 20.00	6	
	ATOM	2282	ō	LEU				97.918	9.614	-3.806	1.00 20.00	8	
	ATOM	2283	N	THR				97.776	9.134	-1.600	1.00 20.00	7	
15	ATOM	2284	CA	THR				97.867	7.678		1.00 20.00	6	
13	ATOM	2285	CB	THR				96.513	7.046	-2.149	1.00 20.00	6	
	ATOM	2286		THR				96.111	7.555	-3.427	1.00 20.00	8	
	ATOM	2287	CG2					95.439	7.355	-1.112	1.00 20.00	6	
			C	THR				98.933	7.238	-2.736	1.00 20.00	6	
20	MOTA	2288		THR				99.903	7.238	-2.730	1.00 20.00	8	
20	MOTA	2289	0							-3.280	1.00 20.00	8	
	ATOM TER	2290	OXT	THR	8	333		98.802	6.121	-3.200	1.00 20.00		
	ATOM	2291	она	TIP	s	1		42.566	19.118	34.302	1.00 15.09		S
	ATOM	2292	OH2		s	2		41.052	32.378	19.857	1.00 15.82		S
25	ATOM	2293	OH2			3		37.014	33.030	17.747	1.00 16.95		s
23	ATOM	2294	OH2			5		45.353	24.370	18.152	1.00 16.85		s
	ATOM	2295		TIP		6		31.896	13.930	33.235	1.00 20.42		S
	ATOM	2296		TIP		7		50.351	22.781	28.249	1.00 21.14		S
	ATOM	2297		TIP		8		45.246	-0.589	-0.734	1.00 17.74		s
30	ATOM	2298			s	11		46.249	-0.348	-8.523	1.00 21.32		s
50	ATOM	2299		TIP		14		45.756	11.148	29.680	1.00 21.94		S
	ATOM	2300	OH2			15		44.273	13.157	34.592	1.00 15.61		s
	ATOM	2300		TIP		17		53.598	3.722	-1.720	1.00 21.45		S
	ATOM	2301		TIP		18		46.049	13.087	31.565	1.00 20.35		S
35	ATOM	2302		TIP		19		53.422	22.401	-3.280	1.00 23.26		S
33	ATOM	2304	OH2			20		34.587	7.922	5.383	1.00 22.58		S
	ATOM	2304		TIP		21		45.053	27.379	19.376	1.00 29.60		S
	ATOM	2305	OH2			23		28.899	36.416	28.633	1.00 31.68		S
	ATOM	2307	OH2	TIP		24		35.531	11.645	-8.219	1.00 23.45		s
40	ATOM	2307		TIP		25		47.364	28.787	19.612	1.00 23.03		S
40	ATOM	2308	OH2			27		48.859	21.588	12.634	1.00 23.76		S
	MOTA	2310	OH2			29		48.805	8.920	23.626	1.00 22.23		S
	ATOM	2311	OH2		s	31		48.619	7.247	10.112	1.00 21.32		S
	ATOM	2312		TIP		34		44.824	28.720	15.621	1.00 25.27	•	S
15		2312		TIP		35	•	26.030	12.634	13.407	1.00 21.61		s
45	MOTA			TIP		36		50.462	19.810	40.066	1.00 25.45		S
	ATOM	2314				37		39.631	23.510	-0.239	1.00 30.88		s
	ATOM	2315		TIP				44.734	42.655	10.346	1.00 30.84		S
	ATOM	2316		-		40		54.653	3.902	1.503	1.00 27.14		s
50	ATOM	2317		TIP		41				39.754	1.00 28.30		s
50	MOTA	2318		TIP		45		45.693	21.923		1.00 25.73		S
	MOTA	2319		TIP		47		47.820	16.413	7.805	1.00 23.73		s
	MOTA	2320		TIP		48		50.292	31.412	29.642	1.00 32.75		s
	MOTA	2321		TIP		49		26.056	16.646	34.827	1.00 29.80		S
•	MOTA	2322		TIP				31.714	10.996	31.855	1.00 24.21		S
55	MOTA	2323		TIP		53		46.108	23.843	-4.299	1.00 24.21		S
	MOTA	2324		TIP				37.645	11.206	34.448	1.00 28.38		S
	ATOM	2325		TIP				26.371	28.513	12.142	1.00 32.08		S
	MOTA	.2326		TIP				33.564	19.700	3.483	1.00 20.20		S
	MOTA	2327	OH2	TIP	S	64		48.295	-0.632	14.280	1.00 32.13		

						•			
	ATOM	2328	OH2 TIP S	65	40.064	26.036	34.324	1.00 24.17	S
	ATOM	2329	OH2 TIP S	66	29.570	3.958	14.729	1.00 28.94	S
•	ATOM	2330	OH2 TIP S	72	60.085	11.604	6.814	1.00 38.35	s
	ATOM	2331	OH2 TIP S	73	39.203	44.403	18.686	1.00 26.61	· s
5	MOTA	2332	OH2 TIP S	76		12.366	27.366	1.00 28.51	s
	ATOM	2333	OH2 TIP S	8 o	•	33.771	33.329	1.00 28.82	S
	ATOM	2334	OH2 TIP S			13.106	2.128	1.00 40.62	S
-	ATOM	2335	OH2 TIP S			34.381	32.043	1.00 19.35	s
	ATOM	2336	OH2 TIP S			40.331	19.200	1.00 13.33	S
10	ATOM	2337	OH2 TIP S			-0.832	-6.556	1.00 24.11	S
	ATOM	2338	OH2 TIP S		·	28.336	33.481	1.00 27.64	S
	ATOM	2339	OH2 TIP S			-7.101	-7.995	1.00 27.04	S
	ATOM	2340	OH2 TIP S			4.387	19.370	1.00 24.33	
	ATOM	2341	OH2 TIP S			11.549	33.898	1.00 28.02	S
15	ATOM	2342	OH2 TIP S			24.831	1.168	1.00 29.40	s
	ATOM	2343	OH2 TIP S		-	4.952	-6.749		s
	ATOM	2344	OH2 TIP S			27.986		1.00 28.00	S
	ATOM	2345	OH2 TIP S		49.942	24.366	11.558	1.00 29.24	S
	ATOM	2346	OH2 TIP S				30.265	1.00 31.61	S
20	ATOM	2347	OH2 TIP S			7.113	-8.298	1.00 31.57	s
20	ATOM	2348	OH2 TIP S			19.957	-8.378	1.00 26.95	S
	ATOM	2349	OH2 TIP S			22.446	39.624	1.00 40.57	s
	ATOM				45.359	7.052	13.052	1.00 26.27	s
	ATOM	2350	OH2 TIP S		37.150	32.340	32.346	1.00 34.45	S
25	ATOM	2351	OH2 TIP S		43.465	40.457	8.240	1.00 40.48	S
23	ATOM	2352	OH2 TIP S		36.644	8.257	13.418	1.00 30.70	S
	ATOM	2353	OH2 TIP S		41.912	-8.974	-8.264	1.00 26.08	S
	ATOM	2354	OH2 TIP S	124	62.424	15.800	-7.411	1.00 24.08	S
	ATOM	2355 2356			37.266	18.656	-9.097	1.00 28.99	S
30			OH2 TIP S		43.129	26.845	14.606	1.00 25.19	S
30	ATOM	2357	OH2 TIP S		36.339	32.639	29.802	1.00 29.25	S
	MOTA	2358	OH2 TIP S		54.051	14.561	26.498	1.00 33.93	S
	ATOM	2359	OH2 TIP S		41.805	-4.242	5.492	1.00 33.72	S
	MOTA	2360	OH2 TIP S		38.873	25.163	36.697	1.00 30.69	S
35	MOTA	2361	OH2 TIP S		28.777	8.553	25.307	1.00 31.43	S
33	ATOM	2362	OH2 TIP S		53.672		-12.803	1.00 33.45	S
	ATOM	2363	OH2 TIP S		59.892	15.434	11.467	1.00 31.39	S
	ATOM ATOM	2364	OH2 TIP S		31.040	12.361	35.470	1.00 34.07	S
	ATOM	2365				14.292	-0.598	1.00 40.68	s
40	ATOM	2366	OH2 TIP S		46.918	8.748	11.662	1.00 29.23	s
40	ATOM	2367	OH2 TIP S		46.297	-7.287	-9.196	1.00 42.20	S
	MOTA	2368	OH2 TIP S	142	58.193	6.715	-4.685	1.00 35.48	S
	ATOM	2369	OH2 TIP S	143	44.598	4.435	12.503	1.00 27.68	S
	ATOM	2370	OH2 TIP S		27.003	5.999	12.450	1.00 36.30	s
45		2371		145	43.676	32.852	35.735	1.00 35.70	S
43	MOTA	2372	OH2 TIP S		35.783	18.628	36.452	1.00 34.62	S
	ATOM	2373	OH2 TIP S		25.402	4.058	20.638	1.00 45.03	S
	ATOM	2374	OH2 TIP S		45.839	35.853	33.724	1.00 35.47	S
	ATOM	2375	OH2 TIP S		22.176	18.976	16.752	1.00 31.87	S
50	MOTA	2376	OH2 TIP S		43.986	33.179	10.162	1.00 37.70	S
50	ATOM	2377	OH2 TIP S		50.653	20.347	42.428	1.00 35.80	S
	ATOM	2378	OH2 TIP S		47.843	24.314	9.506	1.00 31.05	S
	ATOM	2379	OH2 TIP S		44.693		-14.175	1.00 29.90	s
	ATOM	2380	OH2 TIP S		26.560	36.851	31.684	1.00 49.29	S
	ATOM	2381	OH2 TIP S			8.019		1.00 29.21	S
55	ATOM	2382	OH2 TIP S		30.432	28.741	12.438	1.00 37.76	S
	ATOM	2383	OH2 TIP S		41.004	20.553	6.423	1.00 39.53	S
	ATOM	2384	OH2 TIP S		49.258	20.069	29.294	1.00 33.97	s
	ATOM	2385	OH2 TIP S		48.082	28.459	16.489	1.00 33.10	S
	MOTA	2386	OH2 TIP S	161	47.448	18.625	27.683	1.00 34.87	S

	MOTA	2387	OH2 TI	P S	162	19	.687	20.632	23.411	1.00	35.01		s
	ATOM	2388	OH2 TI	P S	163	32	.402	-1.266	22.443		37.26		s
	ATOM	2389	OH2 TI	P S	164	39	.475	33.468	33.237		35.34		S
	ATOM	2390	OH2 TI	P S	165	44	.277	18.950	5.162		45.14		s
5	ATOM	2391	OH2 TI	P S	166	34	.797	30.523	10.736		47.55		S
	ATOM	2392		P S	167		.541		-14.949		26.54	,	s
	ATOM	2393	OH2 TI				.333	16.371	1.539		38.68		s
	MOTA	2394	OH2 TI				.761	38.936	27.403		34.66		s
	ATOM	2395		P S			.163	13.264	11.375		41.23		s
10	ATOM	2396	OH2 TI				.459	15.018	31.951		38.11		S
	ATOM	2397	OH2 TI				.261	23.193	40.004		48.96		S
	ATOM	2398	OH2 TI				.924	-0.026	13.224		39.55		S
	ATOM	2399	OH2 TI				.384	37.389	32.543		40.74	•	S
	ATOM	2400	OH2 TI				.394	35.312	27.150		44.33		
15	ATOM	2401	OH2 TI										S
13	ATOM	2401		PS			.066	29.942	34.359		41.46		S
							.354	19.467	7.273		34.56		S
	ATOM	2403	OH2 TI				.298	17.029	31.863		47.74		S
	ATOM	2404		P S			.071	25.027	4.669		43.87		S
20	ATOM	2405	OH2 TI		183		.581	7.487	18.691		41.75		S
20	ATOM	2406	OH2 TI				.269	7.011	-1.891		48.84		S
	ATOM	2407		P S			.234	0.494	6.833		48.16		S
	ATOM	2408	OH2 TI					14.658	19.211		45.27		S
	ATOM	2409	OH2 TI				.341	22.698	42.272		42.20		S
	MOTA	2410	OH2 TI				.292	18.260	-8.097		45.21		s
25	ATOM	2411	OH2 TI				.152	10.606	2.819		40.38		S
	MOTA	2412	OH2 TI				.626	12.619	23.191		34.27		s
	ATOM	2413			193	• 59	.876	11.603	1.216	1.00	46.54		S
	ATOM	2414	OH2 TI	P S	194	57	.592	21.183	-10.646	1.00	45.82		s
	ATOM	2415	OH2 TI	P S	195	31	.509	36.649	21.499	1.00	38.73		S
30	MOTA	2416	OH2 TI	P S	197	50	.270	-1.543	-6.136	1.00	42.66	•	s
	ATOM	2417	OH2 TI	P S	198	24	.467	8.729	13.088	1.00	42.78		S
	ATOM	2418	OH2 TI	P S	199	38	.098	8.699	25.759	1.00	32.80		S
	ATOM	2419	OH2 TI	P S	200	57	.831	11.358	-13.255	1.00	45.31	•	S
	ATOM	2420	OH2 TI	P S	201	23	.888	22.328	30.524	1.00	37.12		s
35	MOTA	2421	OH2 TI	P S	202	47	.691	26.068	37.666	1.00	37.92		S
	ATOM	2422	OH2 TI	P S	203	38	.653	7.070	29.307	1.00	50.54		S
	ATOM	2423	OH2 TI	P S	206	44	.424	27.583	2.092	1.00	53.50		S
	ATOM	2424	OH2 TI	P S	212	22	.258	2.296	17.948	1.00	47.38		s
	ATOM	2425	OH2 TI	P S	214	19	.843	17.943	23.303	1.00	30.36		S
40	ATOM	2426	OH2 TI	P S	216	27	.647	11.344	24.681	1.00	31.32		s
	ATOM	2427	OH2 TI	P S	217	37	.953	7.817	-9.284	1.00	45.97		S
	ATOM	2428	OH2 TI	P S	218	33	.845	34.040	12.124	1.00	38.11		s
	ATOM	2429	OH2 TI	P S	219	58	.484	15.269	13.717	1.00	38.26		S
	ATOM	2430	OH2 TI	P S	220	48	.526	40.920	26.583	1.00	35.23		s
45	ATOM	2431	OH2 TI	P S	222	52	.094	21.184	38.122	1.00	29.86		s
	ATOM	2432	OH2 TI				.889	5.881	3.281		37.63		s
	ATOM	2433	OH2 TI				.642		-10.684	1.00	34.89		s
	ATOM	2434	OH2 TI				.284	2.916	19.133		34.10		s
	ATOM	2435	OH2 TI				.468		-15.039		37.98		s
50	ATOM	2436	OH2 TI					22.832	21.831		41.57		s
	ATOM	2437	OH2 TI					12.689	14.880		50.22		s
	ATOM	2438	OH2 TI				.102	9.176	5.655		40.57		s
	ATOM	2439	OH2 TI				.618		-11.925		50.71		S
	ATOM	2440	OH2 TI				.822	25.342	19.945		34.93		S.
55	ATOM	2441	OH2 TI				.831	32.218	28.901		37.69		S
	MOTA	2442	OH2 TI				.045	10.774	16.992		39.57		s
	MOTA	2443	OH2 TI				.019	19.850	15.679		41.42		s
	ATOM	2444	OH2 TI				.490	20.949	26.114		34.55		s
	ATOM	2445	OH2 TI				.187	26.377	7.346		39.68		s

	ATOM	2446	OH2 TIP	S 241	33.680	38.342	19.389	1.00 48.93	s
	ATOM	2447	OH2 TIP	S 242	51.539	31.612	10.881	1.00 55.65	S
	MOTA	2448	OH2 TIP	S 244	25.872	14.431	30.404	1.00 46.69	S
	MOTA	2449	OH2 TIP	S 248	37.332	5.849	9.544	1.00 43.81	S
5	MOTA	2450	OH2 TIP	S 250	39.087	-1.293	-9.655	1.00 42.96	S
	ATOM	2451	OH2 TIP	S 258	23.938	30.000	30.010	1.00 38.89	S
	MOTA	2452	OH2 TIP	S 259	24.949	29.749	32.578	1.00 40.17	S
	ATOM	2453	OH2 TIP	S 260	32.111	17.986	1.918	1.00 48.36	s
	ATOM	2454	OH2 TIP	S 266	21.404	12.876	25.603	1.00 57.17	S
10	ATOM	2455	OH2 TIP	S 269	35.425	36.767	12.550	1.00 30.70	S
	ATOM	2456	OH2 TIP	S 270	52.438	25.529	30.131	1.00 44.85	S
	MOTA	2457	OH2 TIP	S 271	53.299	20.156	36.003	1.00 37.15	S
	MOTA	2458	OH2 TIP	S 272	50.914	6.919	23.723	1.00 43.29	S
	ATOM	2459	OH2 TIP	S 274	31.578	30.795	11.014	1.00 50.15	S
15	MOTA	2460	OH2 TIP	S 275	26.341	7.243	22.447	1.00 39.40	S
	ATOM	2461	OH2 TIP	S 276	60.392	18.195	10.235	1.00 37.91	S
	MOTA	2462	OH2 TIP	S 277	47.355	-9.081	-10.821	1.00 48.18	S
	MOTA	2463	OH2 TIP	S 279	41.304	6.175	-16.647	1.00 38.12	S
	ATOM	2464	OH2 TIP	S 282	33.299	21.620	37.881	1.00 46.29	s
20	ATOM	2465	OH2 TIP	S 283	56.469	26.112	-8.575	1.00 43.71	S
	ATOM	2466	OH2 TIP	S 287	48.382	26.573	7.246	1.00 41.43	S
	MOTA	2467	OH2 TIP	S 288	56.240	7.245	-11.331	1.00 41.79	S
	ATOM	2468	OH2 TIP	S 290	49.060	14.978	28.166	1.00 37.03	s
	MOTA	2469	OH2 TIP	S 291	37.095	44.270	26.442	1.00 45.08	S
25	MOTA	2470	OH2 TIP	S 292	47.814	-0.384	-13.299	1.00 48.60	S
	MOTA	2471	OH2 TIP	S 297	58.081	2.784	-7.841	1.00 41.89	S
	MOTA	2472	OH2 TIP	S 298	36.447	45.321	18.644	1.00 54.91	S
	MOTA	2473	OH2 TIP	S 299	49.029	23.328	1.767	1.00 30.55	S
	ATOM	2474	OH2 TIP	S 301	24.375	13.771	8.634	1.00 48.47	S
30	ATOM	2475	OH2 TIP	S 303	47.904	36.798	28.653	1.00 35.76	S
	MOTA	2476	OH2 TIP	S 305	51.156	40.821	27.172	1.00 43.59	S
	MOTA	2477	OH2 TIP		32.943	28.917	35.227	1.00 42.60	S
	MOTA	2478	OH2 TIP		58.462	28.373	6.251	1.00 46.15	S
	MOTA	2479	OH2 TIP	S 308	41.964	30.940	36.712	1.00 48.26	S
35	ATOM	2480	OH2 TIP	S 313	51.176	-1.922	-3.336	1.00 50.61	S
	ATOM	2481	OH2 TIP	S1001	21.319	36.868	23.805	1.00 36.97	. S
	MOTA	2482		S1002	48.880	32.620	27.617	1.00 44.40	S
	MOTA	2483		S1003	61.880	19.473	11.767	1.00 45.49	S
	MOTA	2484		S1004	52.770	21.424	26.815	1.00 24.43	S
40	ATOM	2485		S1005	35.373	29.094	36.197	, 1.00 35.97	S
	MOTA	2486		S1006	40.815	-6.636	4.389	1.00 43.15	S
	MOTA	2487		S1007	44.953	1.286	11.272	1.00 49.45	S
	ATOM	2488		S1010	21.004	16.168	27.009	1.00 48.51	S
	MOTA	2489		S1011	47.094	41.786	9.243	1.00 50.10	S
45	MOTA	2490	OH2 TIP		32.479	2.978	14.158	1.00 49.47	S
	MOTA	2491	012 GLC		48.557		-12.279	1.00 40.72	G
	ATOM	2492	C11 GLC		48.836		-11.097	1.00 38.05	G
	ATOM	2493	C13 GLC		49.266		-11.476	1.00 38.09	G
	ATOM	2494	014 GLC		49.559		-10.292	1.00 33.99	G
50	MOTA	2495	C15 GLC		48.150		-12.257	1.00 37.32	G
	ATOM	2496	016 GLC		48.574		-12.604	1.00 36.74	G
	MOTA	2497	012 GLC		40.114	-6.634	-6.562	1.00 33.52	G
	ATOM	2498	C11 GLC		38.967	-6.592	-7.404	1.00 31.05	G
<i></i>	MOTA	2499	C13 GLC		37.712	-6.417	-6.552	1.00 31.56	G
55	ATOM	2500	014 GLC		36.554	-6.406	-7.389	1.00 30.70	G
	MOTA	2501	C15 GLC		37.792	-5.109	-5.761	1.00 30.03	G
	MOTA	2502	016 GLC		36.609	-4.961	-4.975	1.00 29.66	G
	MOTA	2503	O12 GLC		44.030	8.243	-13.470	1.00 37.90	G

	ATOM	2505	C13	GLC	G	3		42.747	9.974	-14.579	1.00 39.52	G
	MOTA	2506	014	4 GLC	G	3		41.551		-13.942	1.00 39.39	G
	ATOM	2507	C15	GLC	G	3		42.878		-15.934	1.00 41.43	Ğ
	ATOM	2508	016	GLC	G	. 3		41.736		-16.731	1.00 40.78	G
5	ATOM	2509	012	GLC	G	5		40.556	1.005	2.289	1.00 45.25	G
	MOTA	2510		GLC		5		40.966	2.332	1.960	1.00 40.56	G
	ATOM	2511		GLC		5		40.187	3.327	2.814	1.00 40.36	G
	ATOM	2512		GLC		5		38.791	3.169	2.572	1.00 40.71	G
	ATOM	2513		GLC		5		40.619	4.751	2.464	1.00 40.71	G
10	ATOM	2514		GLC		5		39.885	5.681	3.256	1.00 36.89	G
	ATOM	2515		GLC		6		36.951	22.702	40.046	1.00 53.03	G
	ATOM	2516		GLC		6		37.592	21.583	39.422	1.00 62.46	G
	ATOM	2517		GLC		6		38.104	21.978	38.030	1.00 62.40	G
	ATOM	2518		GLC		6		39.034	23.054	38.168	1.00 61.14	G
15	ATOM	2519		GLC		6		36.948	22.429	37.126	1.00 61.72	G
	ATOM	2520		GLC		6		35.992	21.372	36.960	1.00 58.61	
	ATOM	2521		GLC		7		37.316	0.281	14.299		·G
	ATOM	2522		GLC		7		37.655	-0.758	15.222	1.00 73.45	G
	ATOM	2523		GLC		7		36.592	-1.856		1.00 72.78	G
20	ATOM	2524		GLC		7		35.320	-1.299	15.157 15.498	1.00 72.98 1.00 73.88	G
	ATOM	2525		GLC		7		36.924	-2.989			G
	ATOM	2526		GLC	-	. 7		36.972		16.134	1.00 73.66	G
	ATOM	2527		GLC		8		51.921	-2.493 21.898	17.478 5.908	1.00 75.38	G
	ATOM	2528		GLC		8		52.447	20.871		1.00 62.51	G
25	ATOM	2529			G	8		51.476		5.063	1.00 63.42	G
2.5	ATOM	2530		_	G	8		51.297	20.597 21.794	3.908 3.150	1.00 64.28	G .
	ATOM	2531		GLC	_	8		50.121	20.137		1.00 66.28	G
	ATOM	2532		GLC		8		49.233	19.886	4.448	1.00 64.49	G
	ATOM	2532		GLC	-	10		36.044	37.499	29.523		G
30	ATOM	2534		GLC		10		35.164	36.645	30.259	1.00 56.89 1.00 56.97	G G
50	ATOM	2535			G	10		33.849	36.489	29.494	1.00 56.37	G
	ATOM	2536		GLC		10		33.248	37.772	29.308	1.00 56.11	G
	ATOM	2537		GLC		10		32.900	35.580	30.277	1.00 55.84	G
	ATOM	2538		GLC		10	-	31.674	35.442	29.557	1.00 55.39	G
35	ATOM	2539		ATP		1		46.280	25.658	5.170	1.00 51.49	N
	ATOM	2540	PG	ATP		1		46.464	25.053	3.691	1.00 52.22	. N
	ATOM	2541		ATP		1		47.406	23.911	3.763	1.00 51.41	N
	ATOM	2542		ATP		1		46.794	26.182	2.784	1.00 52.07	N
	ATOM	2543		ATP		1		44.976	24.513	3.344	1.00 51.01	N
40	ATOM	2544	PB	ATP		1		44.560	22.969	3.605	1.00 50.20	N
	ATOM	2545		ATP		1		43.083	22.898	3.669	1.00 49.41	N
	ATOM	2546		ATP		1		45.345	22.474	4.766	1.00 50.34	N
	ATOM	2547		ATP		1		45.070	22.231	2.255	1.00 47.77	N
	ATOM	2548	PA	ATP		1		45.075	20.613	2.121	1.00 42.84	N
45	ATOM	2549	01A	ATP		1		45.547	20.291	0.754	1.00 43.81	N
	ATOM	2550		ATP		1		45.807	20.035	3.270	1.00 45.03	N
	ATOM	2551		ATP		1		43.516	20.223	2.245	1.00 41.73	N
	ATOM	2552		ATP		1		42.528	20.925	1.489	1.00 37.57	N .
	ATOM	2553		ATP		1	-	41.127	20.379	1.776	1.00 39.45	N
50	ATOM	2554		ATP		1		40.907	19.024	1.279	1.00 37.72	Ŋ
	ATOM	2555		ATP		1		40.777	20.321	3.251	1.00 38.48	N
	ATOM	2556		ATP		1		40.360	21.615	3.697	1.00 40.42	N
	ATOM	2557		ATP		1		39.608	19.374	3.270	1.00 37.58	N
	ATOM	2558		ATP		1		38.410	20.076	2.924	1.00 37.38	N
55	ATOM	2559		ATP		1		39.939	18.346	2.173	1.00 35.55	N
	ATOM	2560	И9	ATP		1		40.628	17.156	2.747	1.00 31.76	N
	ATOM	2561	C8	ATP		1		41.864	17.126	3.274	1.00 30.49	N
	ATOM	2562	N7	ATP		1		42.143	15.877	3.667	1.00 29.75	N
	ATOM	2563	C5	ATP	N	1		41.088	15.118	3.390	1.00 27.49	N
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	MOTA	2564	C4	ATP	N	1	40.125	15.925	2.810	1.00	30.02	N
	MOTA	2565	из	ATP	N	1	38.937	15.389	2.431	1.00	27.11	. N
	MOTA	2566	C2	ATP	N	1	38.679	14.085	2.615	1.00	25.62	N
	MOTA	2567	N1	ATP	N	1	39.597	13.283	3.175	1.00	21.76	N
5	ATOM	2568	C6	ATP	N	1	40.800	13.768	3.571	1.00	23.90	N
	ATOM	2569	N6	ATP	N	1	41.698	12.964	4.127	1.00	21.94	N
	MOTA	2570	S	S04	I	1	58.680	8.493	-0.639	1.00	56.05	I
	ATOM	2571	01	S04	I	1	57.956	7.875	0.483	1.00	58.83	I
	ATOM	2572	02	S04	I	1	57.886	9.607	-1.188	1.00	57.04	Ĺ
10	ATOM	2573	03	S04	I	1	58.906	7.478	-1.683	1.00	57.47	I
	ATOM	2574	04	S04	I	1	59.976	9.008	-0.156	1.00	57.51	. I
	ATOM	2575	S	S04	I	2	39.339	4.855	7.057	1.00	84.24	I
	ATOM	2576	01	S04	I	2	39.390	6.175	7.711	1.00	85.02	I
	MOTA	2577	02	S04	I	2	40.101	4.897	5.797	1.00	84.75	I
15	MOTA	2578	03	S04	I	2	37.936	4.506	6.766	1.00	84.94	I
	ATOM	2579	04	S04	I	2	39.931	3.842	7.954	1.00	84.44	I
	ATOM .	2580	s	S04	I	3	38.987	-2.256	3.310	1.00	58.58	I
	ATOM	2581	01	S04	1	3	37.734	-1.675	3.827	1.00	59.11	I
	ATOM	2582	02	S04	I	3	39.460	-1.454	2.172	1.00	59.91	I
20	ATOM	2583	03	S04	I	3	38.743	-3.640	2.866	1.00	60.97	I
	ATOM	2584	04	S04	I	3	40.014	-2.260	4.369	1.00	59.58	I
	ATOM	2585	s	S04	I	4	34.397	5.289	30.981	1.00	64.34	. I
	MOTA	2586	01	S04	I	4	33.627	6.528	30.742	1.00	60.43	I
	ATOM	2587	02	S04	I	4	34.337	4.427	29.782	1.00	60.11	I
25	ATOM	2588	03	S04	I	4	33.816	4.572	32.133	1.00	64.39	I
	MOTA	2589	04	S04	I	4	35.806	5.626	31.277	1.00	63.55	· I
	ATOM	2590	s	S04	I	5	55.074	-6.984	-3.711	1.00	75.40	I
	MOTA	2591	01	S04	I	5	54.657	-7.518	-2.399	1.00	74.66	I
	MOTA	2592	02	S04	Ι	5	54.209	-5.845	-4.065	1.00	74.96	I
30	ATOM	2593	03	S04	I	5	54.950	-8.034	-4.742	1.00	74.22	I
	ATOM	2594	04	S04	I	5	56.477	-6.532	-3.633	1.00	75.15	I
	ATOM	2595	02	P04	P	100	57.362	24.998	13.149	1.00	66.76	P
	MOTA	2596	03	PO4	P	100	59.399	26.166	13.761	1.00	66.89	P
	MOTA	2597	04	P04	P	100	57.761	25.606	15.462	1.00	67.43	P
35	MOTA	2598	01	PO4	P	100	57.264	27.325	13.818	1.00	65.91	P
	ATOM	. 2599	P	P04	P	100	57.947	26.025	14.048	1.00	66.69	P
	END											

Example 5: PDK1 fragments

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We produced constructs for expression of different forms of PDK1 in bacteria. The constructs were either in TRC vectors, pET-15b vector and pGEX expression vector to enable the expression of GST fused N-terminally to PDK1. PDK1 expressed from pGEX 51-556 (ie residues 51 to 556 of PDK1) was found to be highly degraded.

PDK1 protein was also expressed with N-terminal His tags from vector TRC comprising PDK1 sequences 51-556, 51-404 and 1-360, or pET15b 51-404 and tested for expression levels and activity. The expression was generally low, around 0.2 mg/L culture. The specific activity was lower than the His-tagged 51-556 protein purified from baculovirus cells. In the case of PDK1 51-404 expressed from pET-15b construct the level of expression turned out to be very variable. This was probably due to instability of the plasmid since we produced evidence that after a growth of 0.2 units of absorbance, (as measured in a spectrophotometer at 600 nm wavelength) the cells growing faster in the culture were actually not harbouring the plasmid with ampiciline resistance. The instability of the plasmid can be due to toxicity produced by basal expression of PDK1. Although production in bacteria was the theoretical best expression system to avoid heterogeneity due to the different extent of phosphorylation of the different phosphorylation sites in hPDK1, it was found that the protein was either degraded, expressed to low levels, had 5 times less specific activity, or was possibly toxic.

The His-tagged purified PDK1 51-556 protein obtained from baculovirus expression system was homogeneous as depicted by the appearance of one band after by SDS-PAGE analysis of a sample.

Nevertheless, the analysis after isoelectric focussing revealed a large smear of protein covering several units of pH. This analysis suggested that the protein was not homogeneous in terms of its isoelectric point, possibly due to the number of phosphorylation sites which were not homogeneously phosphorylated. This protein did not crystallise.

We purified to homogeneity a truncated His-Myc tagged PDK1 (51-404) which lacks the N-terminal 50 residues and the C-terminal 152 residues which include the PH domain. This protein, produced by a baculovirus expression system, had similar characteristics to the full length wild type PDK1 in terms of its activity towards the peptide substrate T308tide, its activation by the peptide PIFtide, and the binding to PIFtide (as analysed by BiaCore). The purified protein was screened for crystallisation conditions using Hampton Research kits (144 different conditions). Crystallisation conditions were screened with two concentrations of PDK1, in the presence or absence of PIFtide, Staurosporine, at 20°C and in the presence of PIFtide at 4°C. No protein crystals were observed after 6 months, suggesting that this construct was not suitable for forming crystals although all other characteristics were similar to wild type protein.

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The His-Myc PDK1 51-404 purified protein was also subjected to protease treatments in order to obtain a protease-insensitive molecule for increasing the chances of obtaining a shorter, stable variant of PDK1. Different protease treatments were tested. Treatment with Glu-C produced a polypeptide of approximately 38 KDa which was stable. This PDK1 protein was active and lacked the His-tag and part of the Myc-tag, and possibly part of the C-terminal residues. This protein was also set up for crystallography screenings. Some crystals were obtained using this preparation after 4 months, but they were not followed up.

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A protein kinase corresponding to residues PDk1 51-387 was also produced, in an identical vector to that used to produce the protein PDK1 51-359. Interestingly, this protein was similar to wild type and PDK1 51-404, but had extreme problems for concentration using conventional methods. The protein could not be concentrated further than 2.5 mg/ml, and no crystals were obtained using this construct.

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The PDK1 protein that finally crystallised is lacking the first 50 aminoacids and was constructed to end at position 359. This protein was stable in the absence of the PH domain and aminoacids that in hPDK1 link the catalytic domain with the PH domain. The construct PDK1 51-359 was also short enough that no other described phosphorylation sites besides activation loop phosphorylation site 241 were present.

15 Example 6: Structural basis for UCN-01 specificity and PDK1 inhibition

The staurosporine derivative UCN-01 (7- hydroxyl staurosporine) has been reported to be a potent inhibitor for PDK1 and is currently in clinical trials for the treatment of cancer. Here we report the crystal structures of staurosporine and UCN-01 in complex with the kinase domain of PDK1. We show that although staurosporine and UCN-01 interact with the PDK1 active site in an overall similar manner, the UCN-01 7-hydroxylgroup, which is not present on staurosporine, generates direct and water-mediated hydrogen bonds with active site residues. Inhibition data from UCN-01 tested against a panel of 29 different kinases show a different pattern of inhibition compared to staurosporine. We discuss how these differences in inhibition could be attributed to specific interactions with the additional 7-hydroxyl-group as well as by the size of the 7-hydroxyl-binding pocket. This information could lead to opportunities for structure-based optimisation of PDK1 inhibitors.

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Insulin and growth factor signalling is mediated by the activation of a lipid kinase, phosphatidylinositol-3-kinase (PI3K), which produces the second phosphatidylinositol(3,4,5)trisphosphate messenger molecule (PtdIns(3,4,5)P) [1]. Upon generation of PtdIns(3,4,5)P, 3-Phosphoinositide Dependent protein Kinase-1 (PDK1) and protein kinase B (PKB, also known as Akt) are co-localised at the plasma membrane through interaction of their Pleckstrin Homology (PH) domains with PtdIns(3,4,5)P [2, 3]. PDK1 activates PKB by phosphorylation of its T-loop (Thr308 in PKB) [4, 5]. PDK1 also activates other protein kinases related to PKB, including isoforms of p70 ribosomal S6 kinase (S6K) [6], serum and glucocorticoid responsive kinases (SGK) [7] and p90 ribosomal S6 kinase (Rsk) [8]. These kinases lack PH domains and do not bind PtdIns(3,4,5)P3, and are thought to be activated by a different mechanism, in which the substrates require a priming phosphorylation in a conserved hydrophobic motif (HM) at their Cterminus (reviewed in [9]). This phosphorylation creates a docking motif that specifically interacts with a pocket on the N-terminal lobe of the PDK1 kinase domain (termed PDK1 interacting fragment (PIF) pocket) [10, 11] bringing PDK1 together with its substrate and enabling PDK1 to phosphorylate these kinases in their T-loop, thereby activating them. A significant number of human cancers possess elevated PtdIns(3,4,5)Plevels due to mutations in a number of genes that regulate the production and degradation of this 3-phosphoinositide. One of the most frequently found mutations occurs in the PtdIns(3,4,5)P 3-phosphatase (PTEN) resulting in constitutive activation of PKB and S6K, which are thought to be major contributors to the proliferation and the survival of such tumour cells [12]. Thus, inhibitors of PDK1 have the potential to act as anti-cancer agents as they would be expected to suppress activation of S6K and PKB and inhibit cell growth and induce apoptosis of cancer cells that possess elevated levels of PtdIns(3,4,5)P.

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PDK1 consists of an N-terminal kinase domain and a C-terminal PHdomain [13]. The structure of the PDK1 kinase domain has been solved (see the preceding Examples and [11]) and leads to a definition of the residues lining the ATP binding site and an understanding of the PDK1 activation mechanism. The PIFbinding pocket could be identified, together with a specific pocket for the phosphorylated Ser/Thr residue on the HM of substrate kinases. Staurosporine, a natural product ATP-competitive inhibitor, inhibits many kinases in the low nM range [14], and therefore displays a high cytotoxicity [15]. UCN-01 (7-hydroxyl staurosporine) is a derivative with an additional hydroxyl group on the lactam ring (Fig. 1). It was originally described as a PKC-selective inhibitor isolated from Streptomyces sp. cultures [16], although further studies showed it to be more non-specific [14, 17]. UCN-01 potently inhibits the growth and induces apoptosis of many cancer cells and these effects are thought to be unrelated to PKC inhibition [18, 19]. Due to its anti-tumour activity in vivo and in vitro, UCN-01 is currently undergoing clinical trials with positive effects being reported in the phase 1 studies (reviewed in [19]). Recent reports suggested the cell cycle checkpoint kinase Chk1 [20] and PDK1 [21] may be key targets of UCN-01 in inhibiting the growth of cancer cells, as both kinases are inhibited by UCN-01 in the low nM range.

Here we report the structures of the PDK1 kinase domain in complex with staurosporine and UCN-01, demonstrating the presence of a pocket that accommodates the 7-hydroxyl group of UCN-01. Specificity tests against a panel of 29 kinases shows that although both staurosporine and UCN-01 are relatively non-specific inhibitors, the fingerprint analysis of UCN-01 inhibition with a panel of protein kinases is significantly different from that of staurosporine. We also perform analysis of residues predicted to line the UCN-01 hydroxyl pocket on a number or protein kinases, and propose a

general model that could account for the different sensitivity of protein kinases for staurosporine and UCN-01.

Methods

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5 Expression, purification and crystallisation

Human PDK1 (residues 51-359) was expressed using a baculovirus mediated infection of the SF21 insect cell line and purified as described in the preceding examples and [11] with the following differences: After elution of the His-tagged protein from the Ni-NTA-agarose beads with 200 mM imidazole, the protein was dialysed against 250 mM NaCl, 25 mM Tris pH 7.5, 1 mM DTT for 3 hours at 4°C. Proteolysis with GST-tagged PreScission protease was performed overnight at 4 °C.

For crystals of the PDK1-UCN-01 complex, 100 µl of PDK1 at a concentration of 6.6 mg/ml was mixed with 30 µl UCN-01 (5.3 mM in 50 % ethanol) and incubated on ice for 2 hours. The protein was crystallized using sitting drop vapour diffusion. 1.25 µl of protein solution was mixed with 0.25 µl cobaltous chloride hexahydrate (0.1 M) and 1 µl mother liquor, consisting of 2.1 M ammonium sulphate, 0.1 M Tris-HCl pH 8.5. Hexagonal, rod-shaped crystals grew at 20 °C and reached a maximum size of 0.05 x 0.05 x 0.3 mm after 7 days. After soaking for 3 seconds in a cryoprotection solution (2.1 M ammonium sulphate, 0.1 M Tris-HCl pH 7.2, 25 % glycerol) crystals were frozen in a stream of cold nitrogen.

PDK1 in complex with staurosporine was crystallized using the hanging drop technique. Drops consisted of 1μ1 PDK1 at 7.6 mg/ml, 1 μl mother liquor (2.1 M ammonium sulphate, 0.1 M Tris- HCl pH 7.2) and 0.25 μl staurosporine (10 mM in DMSO). Hexagonal shaped crystals suitable for

data collection appeared after 6 weeks at 20 C. Crystals were soaked in 1.7 M ammonium sulphate, 0.1 M Tris-HCl pH 7.2, 15% glycerol and frozen in a stream of cold nitrogen.

5 Data collection, structure solution and refinement

Data on the PDK1-staurosporine and PDK1-UCN-01 complexes were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH4. The temperature of the crystals was maintained at 100 K using a nitrogen cryostream. Data were processed using the HKL package [22] with final statistics shown in Table 3. The structures were solved by rigid body refinement with CNS [23] using the previously determined PDK1 structure (See previous Examples; PDB code 1H1W) [11] as a starting model which resulted in an initial R-factor of 0.306 (R $_{\textit{free}} =$ 0.284) for PDK1-staurosporine and 0.299 (R $_{\textit{free}} =$ 0.311) for PDK1-UCN-01. Model building with O [24] and iterative refinement in CNS, including solvent molecules and the T-loop phosphorylation site, resulted in final R-factors as shown in Table 3. The ATP binding site showed well-defined density in the unbiased $|F_o|-|F_c|$, ϕ_{calc} maps for all atoms of staurosporine and UCN-01, including the 7-hydroxyl group (Fig. 8). CNS topologies and coordinates for the inhibitors were generated with PRODRG [25]. No electron density could be observed for residues 51-72 (N-terminus), residues 231-239 (T-loop) and residue 359 (C-terminus) in the PDK1-UCN-01 complex. Residues 51-71 (N-terminus) and 233-238 (Tloop) were disordered in the PDK1-staurosporine complex.

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Determination of inhibition and specificity

Protein kinase assays: PDK1 was assayed for 10 min at 30 °C in a 50 μ l assay mixture in 50 mM Tris pH 7.5, 0.1 mM EGTA, 0.1% 2-

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mercaptoethanol, containing 100 μ M PDK1tide substrate peptide (KTFCGTPEYLAPEVRREPRILSEEEQEMFRDFDYIADWC), 10 mM magnesium acetate, 100 μ M [γ -³²P]ATP (200 cpm/pmole) as described previously [10]. Other protein kinases employed in Table 5, were assayed as described previously [17, 26].

Results & Discussion

Structures of the staurosporine and UCN-01 complexes

PDK1 (residues 51-359) was co-crystallized with staurosporine and UCN-01, and synchrotron diffraction data on a thin hexagonal needle were collected to 2.3 Å and 2.5 Å resolution, respectively.

In the unbiased $|F_o|-|F_c|$, ϕ_{calc} maps well defined (>3.0 σ) density could be observed in the ATP binding site of the kinase, covering all staurosporine/UCN-01 atoms including the 7-hydroxyl group (Fig. 8). After initial rounds of protein model building and inclusion of water molecules, the inhibitor molecules were built and refined with full occupancy to average B-factor of 18.5 Å² (staurosporine) and 17.3 Å²(UCN-01). Further refinement resulted in a final PDK1-staurosporine model with R= 0.218 ($R_{free} = 0.255$) and a final PDK1-UCN-01 model with R = 0.184 ($R_{free} = 0.257$), both with good stereochemistry (Table 3).

The staurosporine molecule is located in the ATP-binding site (which lies between the N-terminal and C-terminal lobes of kinases [27, 28]), at the same position described for the inhibitor in complex with the closely related (38 % sequence identity) protein kinase A (PKA, [29], PDB code 1STC) (Fig. 8). Hydrophobic residues on both sides of the ATP binding cleft sandwich the heterocyclic moiety of staurosporine, namely Leu88, Val96, Ala109, Leu98 (small lobe) and Thr222, Leu212 of the larger lobe (Fig. 1).

Similar to the PKA-staurosporine complex, the lactam group mimics the interactions of the adenine base in ATP with the protein backbone, where 2 conserved hydrogen bonds are formed between the lactam-nitrogen N6 in staurosporine (nomenclature according to [30]) and the backbone-oxygen of Ser160, and the lactam-oxygen at the C5 position and the backbone-nitrogen of Ala162 (Table 4). An additional hydrogen bond is mimicked in the staurosporine sugar-moiety, where the methyl-amino group contacts oxygen O 2 of Glu166, similar to the hydrogen bond with the ribose in the PDK1-ATP complex [11], and also the backbone carbonyl of Glu209 (Table 4).

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The UCN-01 molecule occupies the same position in the ATP binding site as staurosporine (maximum atomic shift = 0.35 Å) (Fig. 9). The same hydrophobic interactions are made to the heterocyclic moiety in the PDK1staurosporine complex. Hydrogen bonding interactions to the heterocycle and the sugar moiety are also conserved, with similar geometry (Table 4). However, the 7-hydroxyl group of UCN-01 forms several novel hydrogen bonds (Fig. 9, Table 4). It hydrogen bonds directly to Oy 1 of Thr222 (Fig. 9, Table 4). In addition, an ordered water molecule (B-factor = 24.0 Å^2) is found in a position where it contacts the 7-hydroxyl (distance = 3.0 Å, Table 4) and the oxygen O_E1 of Gln220 (distance = 2.5 Å) the side chain of which is shifted towards the ligand (1.5 Å for C δ , rotation of 82° around χ_1) compared to the PDK1-STO complex. However, the water molecule is buried in a predominantly hydrophobic pocket, lined by Val143, Leu212 and Cy 2 of Thr222 (Fig. 9). Val143 also changes its position compared to the PDK1-staurosporine complex (Fig. 9), moving further towards the back of the pocket (shift of 0.7 °A for the Cα carbon, and a rotation of 100° around χ_1) and displaces an ordered water molecule present in the PDK1staurosporine complex (Fig. 9), and also observed in other kinasestaurosporine complexes [31, 30]. These changes result in more space to accommodate the bulky 7-hydroxyl group on UCN-01 as indicated by a 6 °A³ increase in ligand volume (calculated with VOIDOO [32]).

Comparison with Chk1-UCN-01

High resolution data for the Chk1 kinase bound to staurosporine and UCN-01 is available (PDB code 1NVQ [30]). In Chk1, Ser147, the equivalent of Thr222 in PDK1, also hydrogen bonds the UCN-01 7-OH directly. In addition, a water mediated network of hydrogen bonds to UCN-01 is observed. However, in Chk1 the water molecule that hydrogen bonds UCN-01 occupies a different position (shifted 5.2 Å compared to the PDK1-UCN-01 complex). Chk1 appears to have a more extended hydrophilic cavity, as there are 2 additional buried water molecules present also in the Chk1-staurosporine complex. The corresponding residue to Gln220 in PDK1 is a Lys (Lys145) in Chk1, which does not interact with the ligand but points away from it.

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UCN-01 inhibition and specificity

PDK1 inhibition by UCN-01 and staurosporine was measured using kinase assays with P^{32} -labelled ATP. PDK1 is inhibited by UCN-01 with an IC₅₀ value of 5 nM, and by staurosporine with an IC₅₀ of 6.5 nM. As a measure for overall specificity of UCN-01 and staurosporine, the effect of these inhibitors was tested against a panel of 29 protein kinases as described previously [17, 26]. The results are shown in Table 5 as percentage of control activity. These data further confirm that UCN-01 and staurosporine are aspecific inhibitors. UCN-01 at 1 μ M concentration reduces the activity of nine kinases in the panel to less than 10%, and of ten others to below 60% of control activity. Staurosporine at 1 μ M will inhibit twelve kinases to less than 10% control activity, and another ten to below 60%. Interestingly, however, several of the protein kinases were differentially inhibited by

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staurosporine and UCN-01 (Table 5). In an attempt to understand these differences the panel of kinases was divided in four distinct classes: (a) similar inhibition, (b) stronger inhibition by staurosporine than by UCN-01, (c) stronger inhibition by UCN-01 than by staurosporine, and (d) no inhibition (Table 5). As the additional 7-hydroxyl group is the only difference in the ligand molecules (Fig. 8), and staurosporine and UCN-01 occupy the same position with similar interactions in the binding site (Fig.9), the residues contacting the extra hydroxyl group were identified for PDK1 and extracted from a sequence alignment of all protein kinases used in the panel (Table 5). A structure-based sequence alignment of known kinase structures was obtained from [33], which was used to validate the sequence-based sequence alignment (Table 5). The nature of the side chains lining the hydroxyl-pocket could provide a partial explanation for the relative difference between UCN-01 and staurosporine inhibition. Two trends can be observed. For the kinases that are inhibited by UCN-01, there appears to be a preference for a side chain capable of hydrogen bonding the 7-hydroxyl in the hydroxyl-pocket. This is in agreement with the presence of a Thr/Ser residue that hydrogen bonds the 7-hydroxyl in the structures of PDK1 (Thr222) and Chk1 (Ser147) bound to UCN-01. Seven out of ten kinases that are hit equally by staurosporine and UCN-01 (group (a)) appear to have a potential hydrogen bonding residue (Table 5). The kinases that are more potently inhibited by UCN-01 than by staurosporine (group (c)) contain a Thr at the Thr222 equivalent position (Table 5). Five out of nine kinases that are inhibited more potently by staurosporine than by UCN-01 (group (b)) lack a potential hydrogen binding partner in the 7-hydroxylpocket (Table 5).

A second trend which appears to determine specificity is the size of the residues lining the hydroxyl-pocket. If the predicted total volume of the residues (calculated with the BL- set of side chain volumes [34]) at the

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positions indicated in Table 5 is set against the activity in the presence of UCN-01, a correlation coefficient of 0.6 is obtained. This suggests that despite inaccuracies in this approach, such as the absence of structural information on precise side chain conformation and water molecules, a weak correlation between predicted hydroxyl pocket volume and UCN-01 inhibition exists. For instance, PKA contains a possible hydrogen bonding partner for UCN-01 (Thr183), but Met134 in the centre of the hydroxyl pocket may leave no space for the extra hydroxyl group (Table 5). A similar arrangement of residues can be observed for MAPKAP-K2 (Table 5). This size dependency may also play a role for the protein kinases neither hit by staurosporine nor UCN-01. The sequence alignment shows that the Val143 and Thr222 equivalent residues are replaced by bulkier Leu or Ile residues in several of the Mitogen Activated Protein Kinase families (Table 5). To investigate the effect of these bulkier side chains on the hydroxyl pocket, we, starting from the PDK1 crystal structure, replaced residues Val143 with Ile and Thr222 with Leu in standard side chain rotamers (in O [24]), which indeed resulted in van der Waals clashes with C7 of staurosporine (shortest distances: 2.8 Å for Leu222, 3.5 Å for Ile143), and may therefore explain the lack of susceptibility towards UCN-01 in the Mitogen Activated Protein Kinase families. CDK2 is inhibited by both staurosporine and UCN-01 similarly, however this kinase lacks a hydrogen bonding partner for the 7-hydroxyl and contains a bulky Phe (Phe80) at the Leu159 equivalent position. In a superposition of CDK2-staurosporine structure [31] with PDK1-UCN-01 (RMSD = 1.3Å on $C\alpha$ atoms) staurosporine is seen to be shifted by 1.2 Å out of the potential hydroxyl pocket due to presence of the bulky Phe80. Interaction of the 7-hydroxyl on UCN-01 was described to be water mediated in CDK2 due to the lack of hydrogen bonding residues [35]. This particular example highlights the limitations of the approach described above. Other examples where none of the described effects account for the observed behaviour are AMPK and

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MSK1. Both MSK1 and SGK1 show the same sequence in their hydroxyl-pocket with Thr406/Thr407, respectively, as potential hydrogen bonding partners, but both were placed in different groups. MSK1 activity is abolished by 1 μ M staurosporine, but shows residual activity (11 %) with UCN-01. SGK1 activity is at 25% of control activity with 1 μ M UCN-01, but twice as high with staurosporine.

Conclusions

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UCN-01 was subjected to a specificity analysis against an in-house panel of 29 protein kinases. Contrary to the suggestions of some previous reports, the data show that UCN-01 is not a specific inhibitor as it inhibited more than half of the tested kinases at significant levels. A direct comparison with staurosporine, however, showed a different pattern of inhibition, and was the subject of further analysis. We have reported the crystal structures of PDK1 in complex with the inhibitors staurosporine and UCN-01. Both inhibitors appear to bind to PDK1 in a similar fashion compared to the Chk1-UCN-01 or PKA-staurosporine [29] complex, with additional hydrogen bonding interactions at the UCN-01 7-hydroxyl group. This moiety is hydrogen bonded directly to Thr222 and indirectly via an ordered water molecule to Gln220. A different water-mediated hydrogen bonding network is also observed in other UCN-01 complexes known to date [35, 30], and might serve as a starting point for further structure-based optimisation. The residues around the 7-hydroxyl group ("hydroxylpocket") were aligned with known kinase structures and kinases sequences. It is apparent that spatial effects in the identified pocket play a key role in determining UCN-01 inhibition, as does the presence of hydrogen bonding partners for the additional hydroxyl group.

Table 3

Details of data collection & structure refinement. Values between brackets are for the highest resolution shell. Crystals were cryo-cooled to 100 K. All measured data were included in structure refinement.

Dataset	Staurosporine	UCN-01
	· · · · · · · · · · · · · · · · · · ·	
Space group	P3 ₂ 21	P3 ₂ 21
Cell dimensions (Å)	a=124.17	a=123.39
	b=124.17	b=123.39
	c=47.31	c=47.12
Resolution range (Å)	25-2.30 (2.38-2.30)	25-2.50 (2.59-2.50)
# Observed reflections	31730 (3091)	68515 (6290)
# Unique reflections	18018 (1794)	14395 (1430)
Redundancy	1.8 (1.7)	4.8 (4.4)
I/σI	7.5 (1.8)	4.5 (2.6)
Completeness (%)	95.8 (95.8)	100.0 (99.9)
R _{merge}	0.096 (0.505)	0.167 (0.688)
R _{cryst} , R _{free}	0.218, 0.255	0.189, 0.257
RMSD from ideal		
geometry	}	
Bonds (Å)	0.007	0.009
Angles (°)	1.7	1.8
B-factor RMSD (Å)	1.5	1.4
(bonded, main chain)		
 protein (Å)	31.5	27.3
 inhibitor (Å)	18.5	17.4

Table 4

Hydrogen bonding between inhibitors and PDK1. Hydrogen bonds between PDK1 and UCN-01 / staurosporine (STO) were calculated with WHAT IF [36] using the HB2 algorithm [37]. This algorithm gives a 0 (no hydrogen bond) to 1 (optimal hydrogen bond) score to reflect hydrogen bond geometry (HB2 column). Donor-acceptor distances are also listed (D-A).

Inhibitor	Protein/H	UCN-01	UCN-01	STO D-A	STO	Comment
	₂ O	D-A (Å)	HB2	(Å)	HB2	
O5	N-	2.8	0.76	3.0	0.81	Conserved
	Ala162					
N6	O-Ser162	2.9	0.80	3.1	0.67	Conserved
N4'	O-	3.2	0.68	3.1	0.39	Conserved
	Glu209					
N4'	Οε2-	2.6	0.63	2.5	0.45	Conserved
	Glu166					
07	Ογ1-	3.0	0.56			7-hydroxyl
	Thr222					
O7	H ₂ O	3.0	0.89			Water
	,	Ì .				mediated to
						(Οε1-
						Gln220)

Table 5

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Comparison of inhibition by UCN-01 vs. staurosporine and hydroxyl pocket-lining residues.

The indicated protein kinases were assayed at 0.1 mM ATP as described previously [17, 26], in the absence or presence of 1µM staurosporine (STO) or UCN-01. Results are presented as percentage of kinase activity compared to that in control incubations. The activity results displayed in the two columns are an average of a triplicate determination. Abbreviations not

Thr40

Val

Leu

Kinase

MSK1

defined in main text: ROCKII, Rho-dependent protein kinase-II; AMPK, AMP-activated protein kinase; MKK1, MAP-kinase kinase-1; PRAK, p38-regulated/activated protein kinase; PHK, phosphorylase kinase; CK2, Casein kinase-2; CHK1, cell cycle checkpoint kinase-1; DYRK, dual specificity tyrosine phosphorylated and regulated kinase; CSK, C-terminal Src kinase. Residues lining the hydroxyl pocket are shown in the last five columns, as derived from a multiple sequence alignment with T-Coffee [38].

UCN-

Kinase	510	01					
Both STO and UCN-01						-	•
inhibit				;	•		
PDK1	5 ± 1	0 ± 1	Met13	Val14	Leu15	Gln22	Thr22
IDKI	J - 1	0 - 1	4	3	9	0	2
CHK1 (1NVQ [<u>30]</u>)	3 ± 1	1 ± 0	Ile '	Val	Leu	Lys14	Ser147
CIRT (1144 Q [<u>50]</u>)	J I	1 ± 0	110	,	200	5	
PKCα	8 ± 2	1 ± 0	Leu	Thr	Met	Lys	Ala
AMPK	0 ± 0	1 ± 1	Leu	Ile	Met	Lys	Ala
PHOS.KINASE (1PHK [39])	2 ± 3	1 ± 2	Leu	Ile	Phe	Lys	Thr
Lck (1QPJ [<u>40]</u>)	0 ± 0	3 ± 1	Met	Val	Thr	Lys	Ala
GD770/ 1' 4 (14 O1 F017)	12 ±	0.1.0	Υ	X7-1	DL - 00	T	Ala
CDK2/cyclin A (1AQ1 [31])	12	8 ± 0	Leu	Val	Phe80	Lys	Aua
PKBΔPH (1O6K [<u>41]</u>)	8 ± 2	9 ± 1	Leu	Thr	Met	Lys	Thr
ROCK-II	9 ± 5	13 ± 2	Met	Val	Met	Lys	Ala
S6K1	24 ± 8	21 ± 4	Leu	Val	Leu	Lys	Thr
GSK3β (1I09 [<u>42]</u>)	29 ± 6	25 ± 5	Met	Val	Leu	Lys	Cys
STO inhibits stronger than	1	•					
UCN-01							

 $1 \pm 0 \ 11 \pm 0 \ \text{Leu}$

Val

					6
DYRK1α	2 ± 2 15 ± 2 Leu	Met	Phe	Lys	Val
PKA (1STC [<u>29]</u>)	4±1 27±2 Leu	Val	Met13	Gln	Thr18
MKK1	5 ± 8 53 ± 1 Leu	Val	Met	Lys	Cys
MAPKAP-K2	$23 \pm 1 \ 60 \pm 1 \ \text{His}$	Val	Met	Lys	Thr
CSK (1BYG [<u>43</u>])	$25 \pm 8 \ 58 \pm 3 \ \text{Met}$	Val	Thr	Lys	Ser
SAPK3/p38γ (1CM8 [<u>44]</u>)	37 ± 0 94 ± 8 Leu	Ile	Met	Lys	Leu
SAPK4/p38δ	$40 \pm 5\ 100 \pm 7 \mathrm{Leu}$	Ile	Met	Lys	Leu
PRAK	$48 \pm 1 \ 89 \pm 4 \ His$	Val	Met	Lys	Cys
UCN-01 inhibits stronge	r				
than STO					
MAPKAP-K1a	18 ± 1 ± 1 Leu	Val	Leu	Lys	Thr34 1
SGK1	51 ± 4 22 ± 4 Leu	Val	Leu	Val	Thr40
Neither UCN-01 nor STC)				
inhibits	· •				
MAPK2/ERK2 (1ERK [45])	$\frac{100 \pm}{4}$ 107 ± 5 Leu	Ile	Gln	Lys	Cys
JNKSAPK1c	$91 \pm 3 \ 112 \pm 6 \text{Met}$	Ile	Met	Lys	Leu
SAPK2α/p38 (1P38 <u>[46]</u>)	$76 \pm 4\ 107 \pm 5 $ Leu	Ile ·	Thr	Lys	Leu
SAPK2β/p38β2	84 ± 106 ± 4 Leu	Ile	Thr	Arg	Leu
CK2 (1F0Q [<u>47]</u>)	95 ± 4 102 ± 11 Leu	Val	Phe	Arg	Ile
CK1 (1CKI [<u>48]</u>)	95 ± 96 ± 0 Tyr 11	Pro	Met	Tyr	Ile

NEK6

 $109 \pm$ 80 ± 7 Leu Ile Leu Lys Gly 2

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Example 7: Co-ordinates for PDK1 fragment co-crystallised with Staurosporine

```
REMARK coordinates from restrained individual B-factor refinement
     REMARK refinement resolution: 25.0 - 2.30 A
     REMARK starting r= 0.2196 free_r= 0.2545
                      r= 0.2182 free_r= 0.2553
     REMARK final
     REMARK B rmsd for bonded mainchain atoms= 1.536 target= 1.5
     REMARK B rmsd for bonded sidechain atoms= 2.154 target= 2.0
     REMARK B rmsd for angle mainchain atoms= 2.576 target= 2.0 REMARK B rmsd for angle sidechain atoms= 3.220 target= 2.5
 10
     REMARK rweight= 0.1000 (with wa= 2.58634)
     REMARK target= mlf steps= 30
     REMARK sg= P3(2)21 a= 124.172 b= 124.172 c= 47.314 alpha= 90 beta=
     90 gamma= 120
     REMARK parameter file 1 : /dd1/david/projects/MY_CNS/prot.par
     REMARK parameter file 2 : /dd1/david/projects/MY_CNS/sto.par
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : /dd1/david/projects/MY_CNS/glycerol.par
     REMARK molecular structure file: ../generate/alternate.mtf
20
     REMARK input coordinates: ../minimize/minimize.pdb
     REMARK reflection file= ../../1/hkl/cns.hkl
     REMARK ncs= none
     REMARK B-correction resolution: 6.0 - 2.30
25
     REMARK initial B-factor correction applied to fobs :
     REMARK
             B11= -4.525 B22= -4.525 B33=
                                                 9.049
     REMARK B12= -1.949 B13=
                                   0.000 B23=
                                                  0.000
     REMARK B-factor correction applied to coordinate array B:
     REMARK bulk solvent: density level= 0.340909 e/A^3, B-factor=
30
     36.8807 A^2
     REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
     REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
     REMARK theoretical total number of refl. in resol. range:
                                                                        18858
     (100.0%)
     REMARK number of unobserved reflections (no entry or |F|=0):
                                                                          846
     REMARK number of reflections rejected:
         0.0 %)
     REMARK total number of reflections used:
                                                                        18012
     (95.5%)
     REMARK number of reflections in working set:
                                                                        17259
       91.5 % )
     REMARK number of reflections in test set:
                                                                          753
         4.0 %)
45
    CRYST1 124.172 124.172
                                47.314 90.00 90.00 120.00 P 32 2 1
     REMARK FILENAME="bindividual.pdb"
     REMARK DATE:30-Jan-2003 19:44:02
                                                created by user: david
     REMARK VERSION:1.0
     MOTA
               1 CB
                      PRO A 72
                                       64.267 -7.345 13.422 1.00 74.69 A
    MOTA
               2 CG
                      PRO A 72
                                               -8.432 13.027 1.00 74.97 A
                                       63.278
    MOTA
                       PRO A
                              72
               3
                  C
                                       65.866
                                               ~6.007
                                                       12.013
                                                                1.00 73.72 A
    ATOM
               4 O
5 N
                                               -6.002 10.955
                       PRO A
                              72
                                       66.500
                                                                1.00 73.74 A
                                                        11.034
    MOTA
                              72
                       PRO A
                                       64.256
                                               -7.651
                                                                1.00 74.67 A
    MOTA
               6 CD PRO A 72
                                       63.762
                                               -8.901
                                                        11.640
                                                                1.00 75.33 A
55
    MOTA
                                       64.474 -6.639
               7 CA PRO A 72
                                                        12.090 1.00 74.30 A
    MOTA
               8 N
                       GLN A 73
                                       66.329 -5.474
                                                                1.00 72.17 A
                                                        13.141
    ATOM
               9 CA GLN A 73
                                      67.635 -4.829 13.221 1.00 70.49 A
```

	ATOM	10	CB	GLN	Α	73	67.570	-3.424	12.611	1.00	69.71 A
	ATOM	11	CG	GLN	Α	73	66.670	-2.458	13.363		68.72 A
	ATOM	12	CD	GLN		73	66.722	-1.054	12.795	0.00	69.01 A
	ATOM	13	OE:	l GLN	Α	73	67.785	-0.435	12.735		68.92 A
5	ATOM	14	NE	GLN	Α	73	65.571	-0.541	12.376	0.00	68.92 A
	ATOM	15	C	GLN	Α	73	68.057	-4.728	14.683	1.00	69.53 A
	ATOM	16	0	GLN	A	73	67.267	-5.015	15.585	1.00	69.69 A
	ATOM	17	N	PRO	A	74	69.313	-4.321	14.940	1.00	68.34 A
	MOTA	18	CD	PRO	Α	74	70.411	-4.026	13.999	1.00	67.68 A
10	ATOM	19	CA	PRO	Α	74	69.769	-4.204	16.330	1.00	67.15 A
	MOTA	20	CB	PRO	Α	74	71.198	-3.675	16.178		67.56 A
	ATOM	21	CG	PRO	Α	74	71.635	-4.254	14.855	1.00	67.46 A
	ATOM	22	С	PRO	Α	74	68.866	-3.240	17.105		65.27 A
	MOTA	23	0	PRO	A	74	68.496	-2.186	16.584		65.27 A
15	MOTA	24	N	ARG	Α	75	68.506	-3.598	18.337	1.00	62.56 A
	ATOM	25	CA	ARG	Α	75	67.642	-2.730	19.136		59.53 A
•	ATOM	26	CB	ARG	Α	75	67.543	-3.228	20.582		62.40 A
	ATOM	27	CG	ARG	Α	75	66.120	-3.565	21.023		64.22 A
	ATOM	28	CD	ARG	Α	75	66.020	-3.746	22.537		66.65 A
20	ATOM	29	NE	ARG	A	75	64.741	-4.332	22.943		68.76 A
	ATOM	30	ĊΖ	ARG	Α	75	64.390	-4.572	24.204		70.18 A
	ATOM	31	NH1	ARG	Α	75	65.218	-4.272	25.197		70.31 A
	ATOM	32	NH2	ARG	A	75	63.213	-5.125	24.477		71.64 A
	ATOM	33	C	ARG	A	75	68.184	-1.306	19.126		55.61 A
25	ATOM	34	0	ARG	A	75	69.386	-1.082	18.961		55.58 A
	ATOM	35	N	LYS	A	76	67.294	-0.341	19.295		50.06 A
	ATOM	36	CA	LYS	Α	76	67.704	1.050	19.297		45.50 A
	ATOM	37	CB	LYS	A	76	66.498	1.941	19.594		45.42 A
	ATOM	38	ĊĠ	LYS	Α	76	66.404	3.192	18.735		45.70 A
30	ATOM	39	CD	LYS	Α	76	66.329	2.829	17.257		44.53 A
	ATOM	40	CE	LYS	Α	76	66.030	4.045	16.396		44.45 A
	ATOM	41	NZ	LYS	Α	76	66.091	3.733	14.939		43.30 A
	ATOM	42	C	LYS	A	76	68.783	1.251	20.359		42.73 A
	ATOM	43	0	LYS	Α	76	68.715	0.681	21.447		42.46 A
35	ATOM	44	N	LYS	Α	77	69.793	2.046	20.038		39.63 A
	ATOM	45	CA	LYS	A	77	70.851	2.309	20.995		36.33 A
	ATOM	46	CB	LYS	Α	77	72.139	2.670	20.267		36.33 A
	ATOM	47	CG	LYS	Α	77	72.655	1.570	19.353		36.55 A
	ATOM	48	CD	LYS	Α	77	74.005	1.945	18.785		35.61 A
40	ATOM	49	CE	LYS	Α	77	74.491	0.932	17.766		38.34 A
	ATOM	50	NZ	LYS	A.	77	74.706	-0.419	18.354		38.65 A
	ATOM	51	С	LYS	Α	77	70.413	3.459	21.889		35.52 A
	ATOM	52	0	LYS	A	77	69.475	4.190	21.557		32.62 A
	ATOM	53	N	ARG	Α	78	71.097	3.608	23.020		34.95 A
45	ATOM	54	CA	ARG	Α	78	70.801	4.654	23.991		33.79 A
	ATOM	55	CB	ARG		78	69.917	4.094	25.114		35.79 A
	ATOM	56	CG	ARG		78	70.211	2.652	25.483		38.18 A
	ATOM	57	CD .	ARG .		78	69.036	2.040	26.239		38.81 A
	ATOM	58	NE	ARG .		78	68.995	0.578	26.160		38.43 A
50	ATOM	59	CZ	ARG .		78	69.889	-0.232	26.719		38.44 A
	ATOM	60		ARG		78	70.906	0.274	27.401		38.37 A
	MOTA	61		ARG		78	69.760	-1.549	26.610		38.37 A
	ATOM	62	C	ARG		78	72.099	5.230	24.544		31.96 A
	ATOM	63		ARG 2		78	73.133	4.576	24.515		32.75 A
55	ATOM	64		PRO 2		79	72.060	6.470	25.055		30.51 A
	ATOM	65		PRO I		79	70.844	7.272	25.033		27.35 A
	ATOM	66		PRO Z		79	73.236	7.150	25.611		27.35 A 29.82 A
	ATOM	67		PRO 2		79	72.626	8.326	26.365		29.82 A 28.52 A
	ATOM	68		PRO A		79	71.418	8.628	25.559		28.52 A 29.89 A
			-		-			0.020	40.00	±.00 4	OJ A

								•		
	ATOM	69	C	PRO	A.	79	74.129	6.298	26.510	1.00 30.92 A
	ATOM	70	0	PRO	Α	79	75.356	6.357	26.412	1.00 33.32 A
	ATOM	71	N	GLU	Α	80	73.516	5.510	27.383	1.00 29.85 A
	ATOM	72	CA	GLU	A	80	74.273	4.677	28.300	1.00 31.98 A
5	ATOM	73	CB	GLU	A	80	73.327	3.941	29.242	1.00 34 31 A
	ATOM	74	CG	GLU	Α	80	72.697	2.710	28.622	1.00 41.92 A
	ATOM	75	CD	GLU		80	71.205	2.626	28.872	1.00 44.52 A
	ATOM	76		GLU		80	70.461	3.466	28.317	1.00 46.38 A
	MOTA	77	OE2	GLU	A	80	70.780	1.721	29.625	1.00 46.03 A
10	MOTA	78	С	GLU	A	80	75.157	3.663	27.578	1.00 30.62 A
	MOTA	79	0	GLU		80	76.101	3.144	28.170	1.00 30.21 A
	MOTA	80	N	ASP		81	74.859	3.378	26.312	1.00 28.14 A
	MOTA	. 81	CA	ASP	A	81	75.659	2.417	25.548	1.00 27.32 A
	MOTA	82	CB	ASP		81	74.938	1.990	24.253	1.00 27.75 A
15	MOTA	83	CG	ASP		81	73.612	1.275	24.512	1.00 30.45 A
	MOTA	84		ASP		81	73.495	0.549	25.525	1.00 30.76 A
	MOTA	85		ASP		81	72.686	1.424	23.686	1.00 30.74 A
	MOTA	86	C	ASP		81 .	77.026	2.990	25.166	1.00 26.35 A
	ATOM	87	0	ASP		81	77.895	2.266	24.680	1.00 25.33 A
20	MOTA	88	N	PHE		82	77.217	4.283	25.404	1.00 24.95 A
	ATOM	89	CA	PHE		82	78.457	4.948	25.035	1.00 23.57 A
	MOTA	90	CB	PHE		82	78.168	6.040	23.991	1.00 23.02 A
	MOTA	91	CG	PHE		82	77.507	5.534	22.742	1.00 23.64 A
	MOTA	92		PHE		82	78.270	5.059	21.680	1.00 23.15 A
25	MOTA	93		PHE		82	76.123	5.504	22.640	1.00 23.41 A
	MOTA	94		PHE		82	77.670	4.559	20.540	1.00 23.43 A
	MOTA	95	CE2	PHE		82	75.504	5.003	21.498	1.00 24.29 A
	MOTA	96	CZ	PHE		82	76.283	4.527	20.444	1.00 25.15 A
	ATOM	97	C	PHE		82	79.199	5.609	26.186	1.00 24.39 A
30	MOTA	98	0	PHE		82	78.647	5.847	27.259	1.00 22.78 A
	MOTA	99	N	LYS		83	80.471	5.896	25.932	1.00 22.40 A
	ATOM	100	CA	LYS		83	81.294	6.615	26.869	1.00 23.38 A
	ATOM	101	CB	LYS		83	82.554	5.834	27.250	1.00 24.29 A
25	MOTA	102	CG	LYS		83	83.453	6.594	28.227	1.00 27.32 A
35	MOTA	103	CD	LYS		83	84.411	5.675	28.988	1.00 31.40 A
	ATOM	104	CE	LYS		83	85.321	4.906	28.044	0.00 30.06 A
	ATOM	105	NZ	LYS		83	86.145	5.819	27.207	0.00 30.54 A 1.00 24.47 A
	ATOM	106	C	LYS		83	81.656	7.847	26.046 25.162	1.00 24.47 A
40	ATOM	107	0	LYS		83	82.518	7.787	26.309	1.00 20.05 A
40	ATOM	108	И	PHE		84 84	80.965 81.211	8.951 10.182	25.583	1.00 21.53 A
	ATOM ATOM	109	CA CB	PHE		84	80.073	11.169	25.811	1.00 21.01 A
		110	CG	PHE		84	78.794	10.757	25.159	1.00 20.02 A
	ATOM	111 112		PHE		84	77.915	9.905	25.805	1.00 20.03 A
45	ATOM ATOM	113		PHE		84	78.498	11.176	23.868	1.00 19.96 A
43		114		PHE		84	76.764	9.473	25.183	1.00 19.47 A
	ATOM ATOM	115		PHE		84	77.346	10.748	23.233	1.00 21.09 A
	ATOM	116	CEZ	PHE		84	76.475	9.894	23.890	1.00 20.64 A
	ATOM	117	C	PHE		84	82.525	10.820	25.966	1.00 22.27 A
50	ATOM	118	0	PHE		84	82.900	10.822	27.129	1.00 24.09 A
50		119	N	GLY		85	83.213	11.371	24.972	1.00 22.72 A
	ATOM ATOM	120	CA	GLY		85	84.496	12.007	25.203	1.00 22.72 A
		121	C	GLY		85	84.540	13.481	24.839	1.00 22.72 A
	ATOM ATOM	121	0	GLY		85	83.622	14.228	25.158	1.00 22.72 A
55	ATOM	123	N	LYS		86	85.608	13.894	24.162	1.00 22.49 A
,,	ATOM	124	CA	LYS		86	85.794	15.291	23.784	1.00 22.53 A
	ATOM	125	CB	LYS		86	87.238	15.530	23.333	1.00 24.44 A
	ATOM	126	CG	LYS		86	87.617	14.804	22.051	1.00 26.94 A
	ATOM	127	CD	LYS		86	89.033	15.120	21.594	1.00 29.52 A
	AZ OFF									

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	MOTA	128	CE	LYS	A	86	89.166	16.571	21.154	1.00 35.93 A
	ATOM	129	NZ	LYS	A	86.	90.505	16.892	20.553	1.00 38.21 A
	ATOM	130	С	LYS	A	86	84.857	15.798	22.699	1.00 23.09 A
	ATOM	131	0	LYS	A	86	84.295	15.032	21.923	1.00 22.85 A
5	ATOM	132	N	ILE	Α	87	84.702	17.114	22.664	1.00 22.28 A
	ATOM	133	CA	ILE	Α	87	83.867	17.780	21.683	1.00 21.22 A
	ATOM	134	CB	ILE		87 .	83.429	19.170	22.204	1.00 22.05 A
	ATOM	135	CG2			87	82.792	19.993	21.076	1.00 17.65 A
	MOTA	136	CG1	ILE		87	82.493	18.998	23.406	1.00 21.65 A
10	ATOM	137		ILE		87	82.159	20.300	24.118	1.00 18.47 A
	ATOM	138	C	ILE		87	84.707	17.963	20.418	1.00 21.83 A
	ATOM	139	ŏ	ILE		87	85.782	18.543	20.470	1.00 21.99 A
	ATOM	140	N	LEU		88	84.226	17.463	19.288	1.00 22.57 A
	ATOM	141	CA	LEU		88	84.964	17.614	18.039	1.00 22.76 A
15	ATOM	142	CB	LEU		88	84.586	16.515	17.044	1.00 20.65 A
	ATOM	143	CG	LEU		88	84.899	15.107	17.535	1.00 20.03 A
	ATOM	144		LEU		88	84.455	14.082	16.502	1.00 20.03 A 1.00 17.42 A
	ATOM	145	CD2	LEU		88	86.392	15.004	17.813	1.00 17.42 A
	ATOM	146	C	LEU		88	84.657	18.964	17.428	1.00 17.70 A 1.00 23.53 A
20	ATOM	147	Õ	LEU		88	85.512	19.577	16.794	1.00 23.33 A 1.00 24.73 A
	ATOM	148	N	GLY		89	83.430	19.428	17.619	1.00 24.73 A 1.00 24.20 A
	ATOM	149	CA	GLY		89	83.057	20.710	17.019	1.00 24.20 A 1.00 28.57 A
	ATOM	150	C	GLY		89	81.649	21.131	17.032	1.00 28.57 A 1.00 32.57 A
	ATOM	151	0	GLY		89	80.834	20.318	17.882	1.00 32.37 A 1.00 32.78 A
25	ATOM	152	N	GLU		90	81.363	22.412	17.882	1.00 32.78 A 1.00 35.17 A
2.5	ATOM	153	CA	GLU		90	80.063	22.964	17.542	
	ATOM	154	CB	GLU		90	80.168	23.853	18.784	1.00 39.17 A 1.00 41.47 A
	ATOM	155	CG	GLU		90	80.112	23.053		
	ATOM	156	CD	GLU		90	80.422	23.893	20.082	1.00 47.18 A 1.00 50.49 A
30	ATOM	157		GLU		90	81.610	24.228	21.313 21.526	1.00 50.49 A
50	ATOM	158	OE2	GLU		90	79.476	24.210	22.067	1.00 51.41 A
	ATOM	159	C	GLU		90	79.436	23.743	16.402	1.00 33.44 A 1.00 40.69 A
	ATOM	160	ō	GLU		90	80.110	24.185	15.471	1.00 40.64 A
	ATOM	161	N	GLY		91	78.121	23.881	16.488	1.00 40.84 A
35	ATOM	162	CA	GLY		91	77.363	24.618	15.503	1.00 42.56 A 1.00 43.40 A
33	ATOM	163	C	GLY		91	76.303	25.335	16.306	1.00 43.40 A
	MOTA	164	0	GLY		91	76.154	25.083	17.507	1.00 44.63 A 1.00 43.64 A
,	MOTA	165	N	SER		92	75.579	26.244	15.669	1.00 43.84 A 1.00 47.22 A
	ATOM	166	CA	SER		92	74.522	26.244	16.366	1.00 47.22 A 1.00 48.94 A
40	ATOM	167	CB	SER		92	73.961	28.066	15.461	1.00 48.94 A 1.00 51.50 A
	ATOM	168	OG	SER		92	73.663	27.541	14.175	1.00 54.98 A
	ATOM	169	C	SER		92	73.454	25.928	16.625	1.00 47.87 A
	ATOM	170	0	SER		92	72.745	25.950	17.635	1.00 47.07 A
	ATOM	171	N	PHE		93	73.392	24.994	15.689	1.00 47.78 A
45	ATOM	172	CA	PHE		93	72.434	23.909	15.697	1.00 46.02 A
	ATOM	173	CB	PHE		93	72.297	23.369	14.263	1.00 40.02 A 1.00 49.54 A
	ATOM	174	CG	PHE		93	73.588	23.398	13.459	1.00 49.34 A
	ATOM	175		PHE		93	74.301	22.229	13:209	1.00 50.29 A
	ATOM	176		PHE		93	74.058	24.593	12.915	1.00 52.29 A 1.00 51.94 A
50	ATOM	177		PHE		93	75.459	22.245	12.424	1.00 51.34 A
50	ATOM	178		PHE		93	75.209	24.622	12.135	1.00 52.28 A
	ATOM	179	CZ	PHE		93		23.443	11.887	1.00 52.58 A 1.00 53.99 A
	ATOM	180	C	PHE		93	75.911 72.700		16.662	
	ATOM	181	0	PHE		93	72.700	22.754 22.245	17.292	1.00 43.48 A 1.00 42.15 A
55	ATOM	182	И	SER		94			16.796	1.00 42.15 A 1.00 39.99 A
	ATOM	183	CA	SER		94	73.955	22.343 21.206	17.655	1.00 39.99 A 1.00 36.12 A
	ATOM	184	CB	SER		94	74.245 73.839	19.937	16.921	1.00 36.12 A 1.00 38.79 A
	ATOM	185	OG	SER		94	74.549	19.863	15.695	1.00 38.79 A 1.00 40.39 A
	ATOM	186	C	SER		94	75.697	21.066	18.083	1.00 40.39 A 1.00 32.29 A
	F3.7014	100		کیدے	- 4		15.091	~T.000	10.003	1.00 32.23 A

										7 00 20 04 B
	ATOM	187	0	SER		94	76.513	21.962	17.890	1.00 30.04 A
	ATOM	188	N	THR	A	95	76.006	19.909	18.655	1.00 28.50 A
	ATOM	189	CA	THR	Α	95	77.350	19.614	19.116	1.00 26.86 A
	MOTA	190	CB	THR	A	95	77.432	19.642	20.652	1.00 27.90 A
5	MOTA	191	OG1	THR	Α	95	76.907	20.882	21.136	1.00 32.56 A
	MOTA	192	CG2	THR	Α	95	78.874	19.502	21.112	1.00 27.77 A
	ATOM	193	C	THR	Α	95	77.757	18.225	18.653	1.00 23.70 A
	ATOM	194	0	THR	A	95	76.971	17.287	18.724	1.00 24.35 A
	MOTA	195	N	VAL	Α	96	78.991	18.100	18.184	1.00 22.75 A
10	ATOM	196	CA	VAL	Α	96	79.505	16.813	17.733	1.00 20.60 A
	ATOM	197	CB	VAL	Α	96	80.139	16.909	16.336	1.00 17.79 A
	ATOM	198	CG1	VAL	Α	96	80.625	15.530	15.898	1.00 18.21 A
	ATOM	199		VAL		96	79.131	17.447	15.344	1.00 13.79 A
	ATOM	200	C	VAL		96	80.566	16.351	18.716	1.00 21.23 A
15	ATOM	201	ō	VAL		96	81.600	17.006	18.889	1.00 22.12 A
13	MOTA	202	N	VAL		97	80.310	15.220	19.362	1.00 22.06 A
	MOTA	202	CA	VAL		97	81.244	14.690	20.345	1.00 24.07 A
	ATOM	204	CB	VAL		97	80.592	14.680	21.743	1.00 24.91 A
		205		VAL		97	79.199	14.124	21.649	1.00 28.97 A
20	MOTA	205		VAL		97	81.422	13.859	22.715	1.00 27.97 A
20	ATOM	207	C	VAL		97	81.748	13.298	20.002	1.00 23.47 A
	MOTA		0	VAL		97	81.017	12.491	19.436	1.00 26.62 A
	ATOM	208		LEU		98	83.007	13.024	20.329	1.00 22.92 A
	ATOM	209	N				83.586	11.713	20.063	1.00 23.27 A
	MOTA	210	CA	LEU		98	85.117	11.777	20.110	1.00 21.94 A
25	MOTA	211	CB	LEU		98		10.495	19.854	1.00 22.83 A
	ATOM	212	CG	LEU		98	85.932	9.924	18.486	1.00 22.03 A
	MOTA	213		LEU		98	85.606	10.802	19.945	1.00 23.21 A
	ATOM	214		LEU		98	87.422	10.802	21.144	1.00 23.95 A
	ATOM	215	C	LEU		98	83.069		22.322	1.00 25.03 A
30	ATOM	216	0	LEU		98	83.143	11.099	20.738	1.00 20.02 A
	ATOM	217	N	ALA		99	82.523	9.645	20.736	1.00 23.76 A
	ATOM	218	CA	ALA		99	81.999			1.00 23.76 A 1.00 20.64 A
	MOTA	219	CB .			99	80.485		21.668	1.00 20.64 A
	MOTA	220	C .	ALA		99	82.502		21.357	1.00 26.42 A
35	MOTA	221	0	ALA		99	82.792		20.195	
	ATOM	222	N			100	82.602		22.394	1.00 26.77 A
	ATOM	223	CA			100	83.055		22.238	1.00 26.80 A
	ATOM	224	CB			100	84.362		23.001	1.00 28.29 A
	MOTA	225	CG			100	84.967		22.853	1.00 33.87 A
40	MOTA	226	CD			100	86.281		23.617	1.00 38.01 A
	MOTA	227	NE	ARG	A	100	87.337		22.983	1.00 41.22 A
	MOTA	228	cz			100	87.932		21.837	1.00 41.46 A
	MOTA	229	NH1	ARG	Α	100	87.580		21.190	1.00 41.28 A
	MOTA	230	NH2	ARG	A	100	88.887		21.339	1.00 43.39 A
45	ATOM	231	C	ARG	Α	100	81.970		22.770	1.00 24.32 A
	ATOM	232	0	ARG	Α	100	81.583		23.934	1.00 25.42 A
	ATOM	233	N	GLU	Α	101	81.456		21.900	1.00 22.41 A
	ATOM	234	CA	GLU	A	101	80.417	2.367	22.281	1.00 22.87 A
	ATOM	235	CB	GLU	Α	101	79.787	1.775	21.025	1.00 21.96 A
50	ATOM	236	CG	GLU	Α	101	78.819	0.652	21.292	1.00 24.68 A
	ATOM	237	CD	GLU	Α	101	78.203	0.137	20.018	1.00 28.27 A
	ATOM	238		GLU			78.965	-0.113	19.057	1.00 28.96 A
	MOTA	239		GLU			76.963	-0.022	19.971	1.00 29.77 A
	ATOM	240	C			101	81.015		23.151	1.00 23.59 A
55	ATOM	241	ō			101	81.945		22.738	1.00 24.80 A
	ATOM	242	N			102	80.475		24.351	1.00 26.09 A
	ATOM	243	CA			102	80.982	0.083	25.289	1.00 28.74 A
	MOTA	244	СВ	LEU	Α	102	80.173	0.110	26.593	1.00 30.16 A

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	ATOM	245	CG	LEU	Α	102	80.347	1.308	27.532	1.00 34.19 A
	ATOM	246	CD1	LEU	A	102	81.824	1.692	27.599	1.00 33.27 A
	ATOM	247	CD2	LEU	Α	102	79.52 7	2.477	27.046	1.00 34.46 A
	ATOM	248	С	LEU	A	102	81.042	-1.359	24.791	1.00 28.32 A
5	ATOM	249	0	LEU	Α	102	82.067	-2.024	24.916	1.00 29.83 A
	ATOM	250	N	ALA	Α	103	79.948	-1.841	24.226	1.00 27.34 A
	ATOM	251	CA	ALA	Α	103	79.887	-3.218	23.763	1.00 27.81 A
	ATOM	252	CB	ALA	A	103	78.466	-3.549	23.367	1.00 27.48 A
	ATOM	253	С	ALA	Α	103	80.828	-3.593	22.624	1.00 27.42 A
10	ATOM	254	0	ALA	A	103	81.172	-4.765	22.463	1.00 28.68 A
	ATOM	255.	N	THR	Α	104	81.257	-2.612	21.842	1.00 24.97 A
	ATOM	256	CA	THR	Α	104	82.105	-2.907	20.695	1.00 23.79 A
	ATOM	257	CB	THR	Α	104	81.441	-2.472	19.393	1.00 22.01 A
	ATOM	258	OG1				81.355	-1.041	19.379	1.00 23.91 A
15	ATOM	259		THR	Α	104	80.051	-3.069	19.261	1.00 17.30 A
	ATOM .	260	C	THR			83.444	-2.221	20.712	1.00 25.00 A
	ATOM	261	Ō	THR			84.350	-2.616	19.972	1.00 25.02 A
	ATOM	262	N	SER			83.551	-1.172	21.525	1.00 24.89 A
	MOTA	263	CA	SER			84.775	-0.394	21.616	1.00 24.55 A
20	MOTA	264	CB	SER			85.979	-1.334	21.732	1.00 26.36 A
20	ATOM	265	OG.	SER			87.143	-0.621	22.090	1.00 32.45 A
	MOTA	266	C	SER			84.916	0.514	20.374	1.00 23.38 A
	ATOM	267	ō	SER			85.931	1.175	20.188	1.00 24.92 A
	MOTA	268	N	ARG			83.888	0.546	19.531	1.00 20.51 A
25	MOTA	269	CA	ARG			83.906	1.372	18.323	1.00 19.31 A
23	MOTA	270	CB	ARG			82.778	0.947	17.370	1.00 19.05 A
	ATOM	271	CG	ARG			83.099	-0.283	16.520	1.00 15.69 A
	ATOM	272	CD			106	81.853	-0.804	15.832	1.00 19.45 A
	ATOM	273	NE	ARG			82.144	-1.838	14.846	1.00 20.98 A
30	ATOM	274	CZ	ARG			81.234	-2.673	14.354	1.00 21.77 A
50	ATOM	275		ARG			79.974	-2.599	14.7.68	1.00 19.65 A
•	ATOM	276		ARG			81.577	-3.560	13.427	1.00 21.43 A
	ATOM	277	C			106	83.760	2.858	18.624	1.00 17.84 A
	ATOM	278	o			106	83.022	3.234	19.525	1.00 15.87 A
35	ATOM	279	N			107	84.463	3.691	17.863	1.00 18.23 A
33	ATOM	280	CA			107	84.395	5.144	18.039	1.00 22.75 A
	ATOM	281	CB			107	85.773	5.800	17.929	1.00 23.58 A
	ATOM	282	CG			107	86.828	5.254	18.859	1.00 32.15 A
	MOTA	283	CD			107	88.066	6.131	18.878	1.00 35.04 A
40	ATOM	284		GLU			88.145	7.019	19.755	1.00 36.99 A
40	ATOM	285		GLU			88.949	5.944	18.007	1.00 37.54 A
	ATOM	286	C			107	83.514	5.787	16.982	1.00 21.00 A
	ATOM	287	Ö			107	83.709	5.577	15.787	1.00 21.37 A
	ATOM	288	N			108	82.570	6.593	17.437	1.00 19.48 A
45		289	CA	-		108	81.652	7.298	16.559	1.00 18.30 A
45	MOTA	290	CB			108	80.228	6.791	16.754	1.00 17.52 A
	MOTA	291	CG			108	79.993	5.373	16.309	1.00 22.75 A
	MOTA	292	CD1			108	79.727	5.075	14.972	1.00 20.94 A
	ATOM		CE1			108	79.492	3.765	14.571	1.00 23.91 A
50	MOTA	293	CD2			108	80.019	4.324	17.231	1.00 19.41 A
50	ATOM	294	CE2			108	79.788	3.026	16.845	1.00 19.33 A
	ATOM	295	CE2			108	79.780	2.744	15.521	1.00 23.13 A
	ATOM	296					79.333	1.438	15.143	1.00 23.65 A
	ATOM	297	ОН			108 108	81.660	8.777	16.906	1.00 18.00 A
	MOTA	298	C			108	81.929	9.161	18.046	1.00 18.12 A
55	ATOM	299	O			109	81.370	9.603	15.912	1.00 17.20 A
	MOTA	300	N			109	81.274	11.036	16.114	1.00 15.30 A
	MOTA	301	CA				81.853	11.784	14.928	1.00 13.44 A
	ATOM	302 303	CB CB			109	79.759	11.704	16.178	1.00 13.11 H
	ΔΥΥOM	403	(:	AUA	А		12.133	11.4VJ	10.1°	

79.056 11.019 15.179 1.00 17.23 A MOTA 304 0 ALA A 109 17.362 1.00 17.40 A 79.250 11.522 305 ILE A 110 MOTA N 1.00 17.60 A ILE A 110 77.814 11.654 17.542 MOTA 306 CA 18.842 1.00 16.56 A 10.957 MOTA 307 CB ILE A 110 77.380 1.00 14.97 A 11.236 19.119 CG2 ILE A 110 75.906 MOTA 308 CG1 ILE A 110 77.672 9.453 18.728 1.00 14.02 A ATOM 309 1.00 11.93 A 19.907 77.197 8.632 CD1 ILE A 110 310 ATOM 13.089 17.548 1.00 19.83 A ILE A 110 77.306 С ATOM 311 13.892 77.690 18.396 1.00 20.84 A ILE A 110 312 0 ATOM 16.597 1.00 18.58 A 13.415 N LYS A 111 76.444 10 ATOM 313 1.00 20.88 A 14.761 16.551 75.902 LYS A 111 ATOM 314 CA 1.00 21.39 A 75.455 15.115 15.131 LYS A 111 CB 315 ATOM 16.558 14.975 1.00 24.84 A CG LYS A 111 75.016 316 MOTA 16.971 1.00 27.43 A 13.516 75.005 CD LYS A 111 MOTA 317 LYS A 111 74.426 18.359 13.343 1.00 28.44 A 318 CE 15 MOTA 1.00 28.27 A 18.871 11.972 LYS A 111 74.619 MOTA 319 ΝZ 17.507 1.00 20.66 A 14.819 74.724 LYS A 111 MOTA 320 C 1.00 20.23 A 14.008 17.410 73.797 LYS A 111 321 0 MOTA ' 15.765 18.441 1.00 20.09 A 74.772 ILE A 112 322 N. MOTA 1.00 23.02 A 73.704 15.914 19.426 ILE A 112 20 MOTA 323 CA 1.00 24.20 A 15.882 20.863 ILE A 112 74.261 CB 324 MOTA 1.00 21.42 A 21.864 15.765 CG2 ILE A 112 73.116 325 MOTA 21.023 1.00 24.14 A 14.692 ILE A 112 75.206 326 CG1 MOTA 22.375 1.00 26.83 A 75.893 14.634 ILE A 112 327 CD1 ATOM 1.00 22.53 A 17.225 19.221 72.962 ILE A 112 328 C 25 **ATOM** 1.00 21.31 A 19.132 ILE A 112 73.573 18.286 MOTA 329 O 1.00 24.04 A 19.150 17.138 71.641 N LEU A 113 330 MOTA 18.940 1.00 25.81 A 70.800 18.313 **LEU A 113** MOTA 331 CA 1.00 24.66 A 17.555 70.135 18.264 **LEU A 113** ATOM 332 CB 1.00 26.73 A 16.295 LEU A 113 70.988 18.095 MOTA 333 CG. 30 1.00 24.51 A 16.093 71.316 16.620 CD1 LEU A 113 334 MOTA 18.637 15.083 1.00 26.16 A 70.234 CD2 LEU A 113 MOTA 335 1.00 27.62 A 19.994 69.702 18.400 336 С **LEU A 113 ATOM** 1.00 29.70 A 17.398 20.314 69.053 LEU A 113 0 MOTA 337 1.00 29.32 A 20.530 69.491 19.597 GLU A 114 ATOM 338 N 35 1.00 31.56 A 21.526 68.445 19.806 **GLU A 114** CA 339 MOTA 1.00 34.85 A 22.391 21.020 68.775 340 CB GLU A 114 MOTA 1.00 42.32 A 21.357 23.392 67.680 CG **GLU A 114** MOTA 341 1.00 45.56 A 24.108 GLU A 114 67.922 22.670 CD MOTA 342 23.417 1.00 48.01 A 23.700 68.086 343 OE1 GLU A 114 MOTA 1.00 48.10 A 67.941 22.673 25.359 **GLU A 114** MOTA 344 OE2 1.00 31.02 A 20.816 GLU A 114 67.107 20.036 С ATOM 345 1.00 30.39 A 20.140 66.926 21.049 GLU A 114 346 0 MOTA 20.967 1.00 30.58 A 19.099 66.176 LYS A 115 MOTA 347 N 1.00 31.63 A 20.321 64.872 19.218 LYS A 115 348 CA 45 MOTA 1.00 28.91 A 63.964 18.049 20.734 349 CB LYS A 115 MOTA 1.00 28.07 A 20.003 64.287 16.742 LYS A 115 350 CG MOTA 1.00 23.95 A 20.368 LYS A 115 63.356 15.580 CD 351 MOTA 21.707 1.00 23.89 A 14.960 63.713 352 CE LYS A 115 MOTA 1.00 24.15 A 13.782 22.020 62.860 LYS A 115 353 NZ 50 MOTA 1.00 33.78 A 20'.591 64.165 20.551 LYS A 115 354 С MOTA 1.00 33.61 A 19.711 LYS A 115 63.495 21.100 355 0 MOTA 1.00 35.55 A 21.076 21.801 64.325 ARG A 116 356 N MOTA 1.00 38.66 A 22.332 22.176 63.682 ARG A 116 357 CA MOTA 1.00 42.20 A 23.663 63.932 22.627 MOTA 358 CB ARG A 116 55 1.00 47.35 A ARG A 116 62.949 23.603 24.302 359 CG MOTA 25.109 1.00 52.44 A 63.670 24.685 360 CD ARG A 116 MOTA 1.00 56.30 A 26.166 64.526 24.141 ARG A 116 361 NE MOTA 1.00 57.97 A 27.423 64.142 23.920 MOTA 362 CZARG A 116

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	ATOM	363	NH1	ARG .	A 116	62.899	24.199	27.808	1.00 58.89 A
	ATOM	364	NH2	ARG .	A 116	65.006	23.420	28.300	1.00 56.55 A
	MOTA	365	С	ARG :	A 116	64.227	23.472	21.323	1.00 37.67 A
	MOTA	366	0	ARG :	A 116	63.474	24.246	20.735	1.00 36.66 A
5	ATOM	367	N	HIS :	A 117	65.550	23.555	21.259	1.00 37.78 A
	ATOM	368	CA	HIS :	A 117	66.236	24.590	20.501	1.00 35.88 A
	ATOM	369	CB		A 117		24.417	20.676	1.00 35.60 A
	ATOM	370	CG		A 117		25.532	20.101	1.00 37.06 A
	ATOM	371		HIS .			25.535	19.134	1.00 38.11 A
10	ATOM	372		HIS.			26.831	20.550	1.00 37.56 A
	ATOM	373		HIS .			27.587	19.886	1.00 38.35 A
	ATOM	374		HIS .			26.825	19.021	1.00 38.67 A
	ATOM	375	C.		A 117	•	24.529	19.024	1.00 34.83 A
	ATOM	376	0		A 117		25.554	18.398	1.00 35.80 A
15.	ATOM	377	N		A 118		23.321	18.474	1.00 33.01 A
10.	ATOM	37B	CA		A 118		. 23.122	17.071	1.00 32.12 A
	ATOM	379	CB		A 118		21.629	16.692	1.00 33.37 A
	ATOM	380	CG2		A 118		21.398	15.312	1.00 33.44 A
	ATOM	381		ILE .			21.168	16.732	1.00 33.47 A
20	ATOM	382		ILE .			19.685	16.479	1.00 35.01 A
20	ATOM	383	C ·		A 118		23.603	16.760	1.00 31.17 A
	ATOM	384	Ö		A 118		24.295	15.774	1.00 29.39 A
	ATOM	385	N		A 119		23.209	17.600	1.00 31.17 A
	ATOM	386	CA		A 119		23.590	17.420	1.00 31.73 A
25	ATOM	387	·CB		A 119		22.896	18.473	1.00 31.45 A
23 .	ATOM	388	CG2		A 119		23.560	18.548	1.00 26.98 A
,	ATOM	389	CG1		A 119		21.409	18.131	1.00 27.55 A
•	ATOM	390	CD1		A 119		20.574	19.205	1.00 26.52 A
	ATOM	391	CDI		A 119		25.100	17.519	1.00 33.53 A
30	ATOM	392	ō		A 119		25.714	16.688	1.00 32.81 A
30	ATOM	393	N		A 120		25.691	18.535	1.00 34.30 A
	ATOM	394	CA		A 120		27.125	18.749	1.00 34.63 A
	ATOM	395	CB		A 120		27.506	20.029	1.00 35.03 A
	ATOM	396	C		A 120		27.889	17.574	1.00 35.68 A
35	MOTA	397	0		A 120		28.938	17.195	1.00 36.85 A
23	ATOM	398	Ŋ		A 121		27.369	16.995	1.00 35.66 A
	ATOM	399	CA		A 121		28.041	15.870	1.00 36.43 A
	ATOM	400	CB		A 121		27.726	15.864	1.00 40.99 A
	ATOM	401	CG		A 121		28.166	17.116	1.00 45.01 A
40	ATOM	402	CD		A 121		29.676	17.205	1.00 48.12 A
-10	ATOM	403		GLU			30.104	18.043	1.00 49.33 A
	ATOM	404	OE2		A 121		30.433	16.451	1.00 49.20 A
	ATOM	405	C.		A 121		27.670	14.512	1.00 34.98 A
	ATOM	406	ŏ		A 121		28.105	13.480	1.00 34.50 A
45	ATOM	407	N		A 122		26.869	14.517	1.00 33.68 A
	ATOM	408	CA		A 122		26.434	13.286	1.00 32.99 A
	ATOM	409	CB		A 122		27.639	12.530	1.00 35.58 A
	ATOM	410	CG		A 122		28.373	13.315	1.00 38.88 A
	ATOM	411		ASN			29.154	14.227	1.00 38.30 A
50	ATOM	412		ASN			28.116	12.970	1.00 38.77 A
50	ATOM	413	C		A 122		25.679	12.367	1.00 31.80 A
	ATOM	414	0.		A 122		25.957	11.172	1.00 30.78 A
	ATOM	415	N		A 123		24.716	12.919	1.00 29.93 A
	ATOM	416	CA		A 123		23.966	12.120	1.00 29.87 A
55	ATOM	417	СВ		A 123		24.016	12.775	1.00 30.75 A
55	ATOM	418	CG		A 123		25.406	12.895	1.00 33.94 A
	ATOM	419	CD		A 123		26.049	11.527	1.00 37.59 A
	ATOM	420	CE		A 123		27.466	11.646	1.00 39.07 A
	ATOM	421	NZ		A 123		28.121	10.310	1.00 41.71 A
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	ATOM	422	С	LYS 2	A 123	64.337	22.514	11.880	1.00 27.38 A
	ATOM	423	0	LYS 2	A 123	65.139	21.745	11.355	1.00 24.93 A
	ATOM	424	N	VAL Z	A 124	63.124	22.132	12.260	1.00 24.22 A
	ATOM	425	CA	VAL 2	A 124	62.716	20.756	12.062	1.00 22.73 A
5	ATOM	426	CB	VAL 3	A 124	61.235	20.559	12.416	1.00 22.36 A
	ATOM	427	CG1	VAL :	A 124	60.794	19.146	12.064	1.00 22.84 A
	ATOM	428	CG2	VAL :	A 124	61.031	20.802	13.905	1.00 20.63 A
	ATOM	429	С	VAL :	A 124	62.981	20.320	10.623	1.00 23.50 A
	ATOM	430	o.		A 124	63.633	19.297	10.385	1.00 21.86 A
10	ATOM	431	N	PRO :	A 125	62.512	21.109	9.639	1.00 23.91 A
	ATOM	432	CD	PRO .	A 125	61.806	22.399	9.725	1.00 24.52 A
	ATOM	433	CA	PRO .	À 125	62.737	20.736	8.239	1.00 24.57 A
	ATOM	434	CB	PRO .	A 125	62.147	21.914	7.464	1.00 23.69 A
	ATOM	435	CG -	PRO .	A 125	61.098	22.450	8.400	1.00 25.18 A
15	ATOM	436	С	PRO .	A 125	64.217	20.520	7.923	1.00 23.84 A
	ATOM	437	Ö	PRO .	A 125	64.568	19.618	7.172	1.00 22.92 A
	ATOM	438	N	TYR .	A 126	65.073	21.353	8.501	1.00 24.86 A
	ATOM	439	CA	TYR	A 126	66.511	21.259	8.274	1.00 28.10 A
	MOTA	440	CB		A 126		22.494	8.859	1.00 32.76 A
20 ·	ATOM	441	CG	TYR	A 126	66.802	23.766	8.146	1.00 39.46 A
	MOTA	442	CD1	TYR	A 126	67.466	24.179	6.987	1.00 42.04 A
	ATOM	443			A 126		25.322	6.292	1.00 43.67 A
	ATOM	444	CD2	TYR	A 126	65.722	24.531	8.597	1.00 42.16 A
	ATOM	445	CE2	TYR	A 126	65.309	25.673	7.909	1.00 43.70 A
25	ATOM	446	CZ	TYR	A 126	65.983	26.062	6.758	1.00 44.51 A
	ATOM	447	ОН	TYR	A 126	65.570	27.183	6.068	1.00 45.30 A
	ATOM	448	С	TYR	A 126	67.115	19.984	8.852	1.00 26.14 A
	ATOM	449	0	TYR	A 126	67.768	19.225	8.141	1.00 26.15 A
	ATOM	450	N	VAL	A 127	66.891	19.756	10.141	1.00 24.35 A
30	ATOM	451	CA	VAL	A 127	67.396	18.568	10.819	1.00 24.93 A
	ATOM	452	CB	VAL	A 127	66.956	18.568	12.296	1.00 24.24 A
	ATOM	453	CG1	VAL	A 127	67.444	17.316	12.997	1.00 23.36 A
	ATOM	454	CG2	VAL	A 127	67.492	19.809	12.979	1.00 21.11 A
	ATOM	455	C	VAL	A 127	66.894	17.290	10.130	1.00 25.81 A
35	MOTA	456	0	VAL	A 12	67.655	16.351	9.903	1.00 25.79 A
	ATOM	457	N	THR	A 128	65.612	17.273	9.793	1.00 25.57 A
	MOTA	458	CA	THR	A 128	64.996	16.136	9.114	1.00 26.36 A
	ATOM	459	CB	THR	A 128	63.486	16.384	8.908	1.00 25.21 A
	MOTA	460	OG1	THR	A 128	62.827		10.181	1.00 29.29 A
40	MOTA	461	CG2	THR	A 12	62.883	15.317	8.043	1.00 25.73 A
	ATOM	462	C	THR	A 12	65.640	15.898	7.748	1.00 26.97 A
	MOTA	463	0	THR	A 12			7.366	1.00 25.68 A
	ATOM	464	N	ARG	A 12	65.854		7.012	1.00 27.23 A
	MOTA	465	CA	ARG	A 12			5.692	1.00 29.37 A
45	MOTA	466	CB	ARG	A 12	66.484	18.282	5.032	1.00 32.35 A
	ATOM	467	CG	ARG	A 12			3.583	1.00 36.81 A
	MOTA	468	CD	ARG	A 12	67.208	•	3.064	1.00 40.45 A
	ATOM	469	NE	ARG	A 12	66.178		3.459	1.00 44.54 A
-	MOTA	470	CZ	ARG	A 12			3.268	1.00 48.21 A
50	ATOM	471	NH1	ARG	A 12	9 64.431		2.681	1.00 50.01 A
	ATOM	472	NH2		A 12			3.668	1.00 47.79 A
	MOTA	473	C		A 12			5.828	1.00 28.98 A
	MOTA	474	0		A 12	a contract of the contract of		5.054	1.00 28.26 A
	ATOM	475	N		A 13			6.822	1.00 29.28 A
55	MOTA	476	CA		A 13			7.057	1.00 30.58 A
	MOTA	477	CB		A 13			8.287	1.00 34.18 A
	MOTA	478	CG		A 13			8.344	1.00 38.81 A
	MOTA	479	CD		A 13			9.702	1.00 41.66 A
	MOTA	480	OEI	GLU	A 13	0 71.946	18.408	10.427	1.00 42.36 A

	ATOM	481	OF2	GLU	7	130	73.771	17.236	10.035	1.00 42.31 A
	ATOM	482		GLU			70.063	14.984	7.273	1.00 30.12 A
			C	GLU			70.861	14.298	6.638	1.00 30.12 A 1.00 29.62 A
	MOTA	483	0							
_	ATOM	484	N	ARG			69.228	14.474	8.173	1.00 29.21 A
5	ATOM	485	CA	ARG			69.215	13.046	8.458	1.00 30.93 A
	ATOM	486	CB	ARG			68.241	12.724	9.601	1.00 32.88 A
	ATOM	487	CG	ARG	Α	131	68.035	11.223	9.795	1.00 36.48 A
	ATOM	488	CD	ARG	А	131	67.069	10.885	10.922	1.00 41.14 A
	ATOM	489	NE	ARG	Α	131	66.859	9.440	11.012	1.00 45.98 A
10	ATOM	490	CZ	ARG	A	131	66.167	8.833	11.974	1.00 48.77 A
	ATOM	491	NH1	ARG	Α	131	65.605	9.546	12.946	1.00 48.39 A
	ATOM	492	NH2	ARG	Α	131	66.045	7.509	11.968	1.00 48.16 A
	ATOM	493	С	ARG	Α	131	68.836	12.226	7.224	1.00 29.97 A
	ATOM	494	0	ARG	A	131	69.398	11.157	6.986	1.00 28.24 A
15	ATOM	495	N	ASP	Α	132	67.889	12.725	6.437	1.00 28.56 A
	ATOM	496	CA	ASP			67.460	11.996	5.251	1.00 29.18 A
	ATOM	497	CB	ASP			66.160	12.583	4.710	1.00 31.39 A
	ATOM	498	CG	ASP			65.005	12.409	5.682	1.00 38.76 A
	MOTA	499		ASP			64.892	11.319	6.283	1.00 40.09 A
20	MOTA	500		ASP			64.206	13.355	5.846	1.00 44.19 A
20			C	ASP			68.510	11.936	4.150	1.00 27.67 A
	ATOM	501		ASP			68.688	10.896	3.522	1.00 27.56 A
•		502	0			•	69.200	13.044	3.909	1.00 27.30 A
	MOTA	503	N	VAL			70.232	13.044	2.886	1.00 25.09 A
25	ATOM	504	CA	VAL					2.742	1.00 25.05 A 1.00 25.26 A
25 -	ATOM	505	CB	VAL			70.859	14.459		1.00 25.26 A 1.00 24.32 A
	ATOM	506		VAL			72.157	14.369	1.961	
	ATOM	507		VAL			69.890	15.390	2.029	1.00 24.76 A
	MOTA	508	C	VAL			71.320	12.076	3.266	1.00 25.33 A
	ATOM	509	0	VAL			71.742	11.270	2.445	1.00 23.59 A
30	MOTA	510	N	MET			71.764	12.138	4.520	1.00 26.01 A
	MOTA	511	CA	MET			72.812	11.243	4.995	1.00 27.63 A
	MOTA	512	CB	MET			73.210	11.576	6.436	1.00 25.11 A
	ATOM	513	CG	MET			74.056	12.834	6.539	1.00 27.52 A
	MOTA	514	SD	MET	Α	134	74.875	13.035	8.132	1.00 28.28 A
35	MOTA	515	CE	MET	A	134	73.545	13.741	9.104	1.00 28.66 A
	MOTA .	516	C	MET	A	134	72.431	9.779	4.901	1.00 28.59 A
,	MOTA	517 .	0	MET	А	134	73.276	8.938	4.599	1.00 31.12 A
	MOTA	518	N			135	71.168	9.467	5.165	1.00 29.14 A
	MOTA	519	CA	SER	Α	135	70.709	8.082	5.090	1.00 31.93 A
40	ATOM	520	CB	SER	Α	135	69.261	7.966	5.558	1.00 32.44 A
	ATOM	521	OG	SER	Α	135	69.112	8.470	6.868	1.00 40.09 A
	ATOM	522	С	SER	Α	135	70.786	7.557	3.668	1.00 31.36 A
	ATOM	523	0	SER	Α	135	71.010	6.374	3.454	1.00 32.23 A
	MOTA	524	N	ARG	A	136	70.597		2.701	1.00 31.66 A
45	ATOM	525	CA	ARG	Α	136	70.602	8.075	1.293	
	ATOM	526	CB	ARG	Α	136	69.798	9.095	0.491	1.00 33.51 A
	ATOM	527	CG	ARG			68.361	9.274	0.962	1.00 38.41 A
	ATOM	528	CD	ARG	Α	136	67.676	10.352	0.137	1.00 40.27 A
	MOTA	529	NE	ARG	A	136	67.850	10.090	-1.288	1.00 42.75 A
50	ATOM	530	CZ			136	67.560	10.953	-2.253	1.00 44.58 A
	ATOM	531		ARG			67.071	12.151	-1.950	1.00 45.74 A
	ATOM	532		ARG			67.771	10.621	-3.522	1.00 43.43 A
	ATOM	533	C			136	71.985	7.946	0.670	1.00 32.09 A
	ATOM	534	o			136	72.113	7.513	-0.474	1.00 32.48 A
55	MOTA	535	N			137	73.019	8.329	1.406	1.00 30.72 A
55	ATOM	536	CA			137	74.371	8.253	0.873	1.00 30.30 A
	ATOM	537	CB			137	75.167	9.508	1.262	1.00 29.84 A
	ATOM	538	CG			137	74.541	10.843	0.831	1.00 30.25 A
		539		LEU			75.488	11.963	1.154	1.00 29.16 A
	MOTA	233		220	••		, 5.400		2.474	

	ATOM	540	CD2	LEU A 137	74.23	10.835	-0.656	1.00 29.68 A
	MOTA	541	С	LEU A 137	75.0	7.006	1.369	1.00 29.52 A
	ATOM	542	0	LEU A 137	75.03		2.553	1.00 31.12 A
	ATOM	543	N	ASP A 138	75.74	6.310	0.453	1.00 27.02 A
5	MOTA	544	CA	ASP A 138	76.40	57 5.087	0.773	1.00 25.70 A
•	ATOM	545	CB	ASP A 138		3.887	0.492	1.00 29.85 A
	MOTA	546	CG	ASP A 138		98 2.567	0.858	1.00 33.94 A
	ATOM	547		ASP A 138		15 2.486	1.949	1.00 34.64 A
	ATOM	548	OD2	ASP A 138			0.058	1.00 35.28 A
10	ATOM	549	C	ASP A 138			-0.127	1.00 24.23 A
10		550	ō	ASP A 136		· •	-1.091	1.00 24.33 A
	MOTA	551	N	HIS A 139		· ·	0.209	1.00 20.89 A
	MOTA	552	CA	HIS A 139			-0.577	1.00 19.30 A
	ATOM	553	CB	HIS A 139			-1.553	1.00 17.75 A
1.5	ATOM			HIS A 133	•		-2.564	1.00 17.45 A
15	MOTA	554	CG	HIS A 139			-3.897	1.00 16.63 A
	ATOM	555					-2.235	1.00 20.01 A
	ATOM	556		HIS A 139			-3.322	1.00 16.89 A
	MOTA	557		HIS A 139			-4.344	1.00 16.94 A
	MOTA	558		HIS A 139			0.352	1.00 19.25 A
20	ATOM	559	С	HIS A 139				1.00 13.23 A 1.00 21.17 A
	MOTA	560	0	HIS A 139			1.388	1.00 21.17 A 1.00 17.84 A
	MOTA	561	N	PRO A 140			-0.021	
	MOTA	562	CD	PRO A 140			-1.243	1.00 16.07 A
	MOTA	563	CA	PRO A 140			0.789	1.00 18.04 A
25	ATOM	564	CB	PRO A 14			0.055	1.00 18.70 A
	ATOM	565	CG	PRO A 14	84.0	61 5.315	-1.365	1.00 19.17 A
	ATOM	566	С	PRO A 14				1.00 19.75 A
	MOTA	567	0	PRO A 14	84.6		1.930	1.00 21.01 A
	ATOM	568	N	PHE A 14	1 83.4	60 8.457	0.192	1.00 20.21 A
30	ATOM	569	CA	PHE A 14	1 83.8	69 9.837	0.389	1.00 20.05 A
	MOTA	570	CB	PHE A 14	1 84.1	49 10.496	-0.964	1.00 20.20 A
	ATOM	571	CG	PHE A 14	1 85.3	33 9.909	-1.686	1.00 20.95 A
	ATOM	572	CD1	PHE A 14	1 86.3	62 9.297	-0.975	1.00 21.45 A
	ATOM	573	CD2	PHE A 14	1 85.4	30 9.983	-3.071	1.00 20.27 A
35	ATOM	574		PHE A 14		76 8.765	-1.635	1.00 22.05 A
	ATOM	575		PHE A 14		41 9.456	-3.743	1.00 20.58 A
	ATOM	576	CZ	PHE A 14		62 8.848	-3.027	1.00 20.58 A
	ATOM	577	C	PHE A 14		81 10.679	1.210	1.00 18.71 A
	MOTA	578	ō.	PHE A 14		11.897	1.300	1.00 19.78 A
40	MOTA	579	N	PHE A 14		03 10.027	1.823	1.00 18.61 A
70	ATOM	580	CA	PHE A 14		15 10.738	2.639	1.00 19.11 A
	MOTA	581	CB	PHE A 14			1.966	1.00 17.36 A
	ATOM	582	CG	PHE A 14			0.750	1.00 19.19 A
	ATOM	583		PHE A 14				1.00 19.44 A
45			CD3	PHE A 14	2 79.6		-0.511	1.00 18.39 A
45	ATOM	584	CDZ	PHE A 14	2 79.2			1.00 20.66 A
	MOTA	585		PHE A 14				
	ATOM	586		PHE A 14				1.00 18.95 A
•	ATOM	587	CZ	PHE A 14				1.00 18.98 A
	ATOM	588	C					1.00 18.39 A
50	ATOM	589	0	PHE A 14				1.00 20.79 A
	ATOM	590	Ŋ	VAL A 14		_		1.00 20.94 A
	MOTA	591	CA	VAL A 14				1.00 20.51 A
	MOTA	. 592	CB	VAL A 14	3 80.			1.00 21.30 A
	MOTA	593		L VAL A 14				1.00 21.30 H
55	MOTA	594	CG:					1.00 15.20 A
	MOTA	. 595	С	VAL A 14				.1.00 23.63 A
	MOTA	596		VAL A 14				1.00 23.64 A
	MOTA	597		LYS A 14	14 79.		_	
	MOTA	598	CA		14 78.	221 7.582	6.990	1.00 24.4/ A
				•				

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	ATOM	599	СВ	LYS	A	144	78.714	6.131	6.869	1.00 25.53 A
	ATOM	600	CG	LYS			77.635	5.061	6.997	1.00 32.25 A
	ATOM	601	CD	LYS			78.240	3:660	6.870	1.00 36.07 A
	ATOM	602	CE	LYS			77.187	2.563	7.033	1.00 38.50 A
5			NZ	LYS			77.791	1.186	7.051	1.00 41.46 A
ر	ATOM	603	C	LYS			77.418	7.744	8.275	1.00 41.40 A
	ATOM	604	0					8.019	9.335	1.00 22.00 A
	ATOM	605		LYS			77.973			1.00 23.10 A 1.00 21.59 A
	ATOM	606	N	LEU			76.104	7.583.		1.00 21.39 A
	ATOM	607	CA	LEU	A		75.224	7.661	9.327	50 21.21 AC1
10	ATOM	608	CB	LEU		145	73.918	8.372		
	MOTA	609	CG	LEU		145	72.843			.50 21.32 AC1
	MOTA	610		LEU		145	73.356			.50 19.59 AC1
	MOTA	611		LEU		145	71.569	8.994		.50 21.45 AC1
	ATOM	612	C	PEA	A	145	74.919	6.215		1.00 21.84 A
15	MOTA	613	0	LEU	Α	145	74.283	5.471		1.00 19.24 A
	ATOM	614	N	TYR	A	146	75.363	5.816		1.00 19.77 A
	ATOM	615	CA	TYR	Α	146	75.143	4.444	11.368	1.00 19.92 A
	ATOM	616	CB	TYR	Α	146	76.326	3.944		1.00 18.05 A
	ATOM	617	CG	TYR	Α	146	77.601	3.803	11.415	1.00 17.64 A
20	MOTA	618	CD1	TYR	Α	146	78.435	4.909	11.203	1.00 18.26 A
	ATOM	619	CE1	TYR	Α	146	79.638	4.782	10.516	1.00 17.33 A
	ATOM	620	CD2	TYR	Α	146	78.000	2.560	10.910	1.00 15.57 A
	ATOM	621	CE2	TYR	Α	146	79.208	2.419	10.215	1.00 17.53 A
	ATOM	622	CZ	TYR	Α	146	80.022	3.535	10.026	1.00 18.78 A
25	ATOM	623	ОН			146	81.224	3.413	9.369	1.00 19.47 A
23	ATOM	624	C			146		4.194		1.00 20.60 A
	ATOM	625	ō			146	73.331	3.100		1.00 21.73 A
	ATOM	626	N			147	73.431	5.192		1.00 20.92 A
	ATOM	627	CA			147	72.239	5.025		1.00 22.59 A
30	ATOM	628	CB			147	72.538	4.063		1.00 22.24 A
50	ATOM	629	CG ·			147	73.708	4.488		1.00 21.88 A
	ATOM	630		PHE			73.607	5.578		1.00 21.93 A
	MOTA	631		PHE			74.936	3.843		1.00 21.57 A
		632		PHE			74.715			1.00 25.21 A
35	ATOM .			PHE			76.051	4.279		1.00 21.30 A
33	ATOM	633					75.942	5.371		1.00 24.23 A
	MOTA	634	CZ			147		6.343		1.00 24.23 A 1.00 23.77 A
	ATOM	635	C			147	71.737	7.352		1.00 23.77 A
	ATOM	636	0			147	72.448	6.324	•	1.00 22.31 A 1.00 25.15 A
40	ATOM	637	N			148	70.501	7.503	•	1.00 25.13 A 1.00 25.99 A
40	ATOM	638	CA			148	69.908			1.00 23.99 A 1.00 27.00 A
	ATOM	639	CB			148	68.953	8.251		1.00 27.00 A 1.00 27.79 A
	ATOM	640		THR			67.850	7.400		1.00 27.79 A 1.00 26.35 A
	ATOM	641	CG2			148	69.660	8.661		
	ATOM	642	C			1,48	69.080	7.055		1.00 26.23 A 1.00 26.46 A
45	MOTA	643	0			148	68.591	5.930		
	ATOM	644	N			149	68.942	7.943		1.00 25.72 A
	ATOM	645	CA			149	68.133	7.662		1.00 25.10 A
	ATOM	646	CB			149	68.789	6.593		1.00 23.02 A
	MOTA	647	CG			149	70.088	7.011		1.00 22.26 A
50	MOTA	648	CD1	PHE	Α	149	70.105	7.794		1.00 20.98 A
	ATOM	649		PHE			71.302	6.587		1.00 21.51 A
	MOTA	650	CE1	PHE	Α	149	71.312	8.151		1.00 22.36 A
	MOTA	651	CE2	PHE	A	149	72.511	6.939	20,288	1.00 21.06 A
•	MOTA	652	CZ	PHE	Α	149	72.519	7.722		1.00 19.46 A
55	MOTA	653	C	PHE	Α	149	67.931	8.974	19.427	1.00 27.05 A
	ATOM	654	0	PHE	Α	149	68.565	9.974	19.096	1.00 27.03 A
	ATOM	655	N			150	67.024	8.984	20.391	1.00 29.18 A
	MOTA	656	CA	GLN	Α	150	. 66.757	10.198	21.133	1.00 31.94 A
	MOTA	657	СВ			150	65.697	11.035	20.409	1.00 32.80 A
			•							

	ATOM	658	CG	GLN .	Α	150		64.385	10.302	20.153	1.00 34.22 A
	ATOM	659	CD	GLN .	A	150		63.340	11.169	19.459	1.00 36.88 A
	MOTA	660	OE1	GLN	Α	150		62.630	11.959	20.098	1.00 37.60 A
	ATOM	661	NE2	GLN .	Α	150		63.248	11.033	18.141	1.00 35.03 A
5	MOTA	662	С	GLN	Α	150		66.269	9.890	22.531	1.00 32.97 A
	MOTA	663	0	GLN .	Α	150		65.857	8.768	22.825	1.00 33.19 A
	ATOM	664	N	ASP	Α	151		66.355	10.890	23.398	1.00 34.27 A
	ATOM	665	CA	ASP	A	151		65.847	10.771	24.753	1.00 35.77 A
	ATOM	666	CB	ASP	Α	151		66.957	10.933	25.796	1.00 35.66 A
10	ATOM	667	CG	ASP	Α	151		67.760	12.194	25.604	1.00 38.11 A
	MOTA	668	OD1	ASP	А	151		67.172	13.216	25.195	1.00 39.31 A
	ATOM	669		ASP				68.982	12.167	25.879	1.00 41.03 A
	ATOM	670		ASP				64.823	11.904	24.838	1.00 36.64 A
	ATOM	671		ASP				64.401	12.428	23.803	1.00 36.42 A
15	ATOM	672	N	ASP				64.427	12.301	26.041	1.00 38.18 A
15	MOTA	673	CA	ASP				63.427	13.357	26.171	1.00 39.81 A
	ATOM	674	CB	ASP				63.022	13.534	27.637	1.00 44.46 A
	ATOM	675	CG	ASP				62.291	12.324	28.186	1.00 50.02 A
	ATOM	676		ASP				61.313	11.876	27.541	1.00 52.36 A
20	ATOM	677		ASP				62.689	11.822	29.263	1.00 52.75 A
20	ATOM	678	C	ASP				63.822	14.709	25.594	1.00 37.45 A
•	ATOM	679	Ö	ASP				62.988	15.408	25.026	1.00 36.81 A
	MOTA	680	Ŋ	GLU				65.091	15.077	25.708	1.00 35.46 A
	ATOM	681	CA	GLU				65.501	16.378	25.211	1.00 33.50 A
25	ATOM	682	CB	GLU				66.132	17.174	26.354	1.00 36.16 A
23		683	CG	GLU				65.389	17.065	27.687	1.00 37.72 A
	MOTA	684	CD	GLU				65.657	15.753	28.402	0.00 37.23 A
	ATOM			GLU			•	65.063	15.530	29.479	0.00 37.39 A
	MOTA	685		GLU				66.464	14.947	27.893	0.00 37.39 A
20	ATOM	686	C	GFA				66.432	16.425	23.995	1.00 31.79 A
30	MOTA	687		GLU			•	66.498	17.451	23.323	1.00 30.80 A
	MOTA	688	0	LYS				67.131	15.334	23.691	1.00 30.35 A
	MOTA	689	N	LYS				68.069	15.357	22.569	1.00 28.14 A
	MOTA	690	CA	LYS				69.505	15.358	23.099	1.00 27.32 A
25	MOTA	691	CB CG	LYS				69.853	16.503	24.026	1.00 29.91 A
35	ATOM	692						71.234	16.302	24.648	1.00 30.14 A
	MOTA	693	CD .	LYS LYS				71.606	17.450	25.592	1.00 32.52 A
	ATOM	694	CE	LYS				72.780	17.121	26.469	1.00 31.90 A
	MOTA	695	NZ	LYS				67.967	14.261	21.515	1.00 26.36 A
40	ATOM	696	C	LYS	-			67.517	13.145	21.781	1.00 23.71 A
40	MOTA	697	0	LEU				68.413	14.610	20.311	1.00 24.76 A
	MOTA	698	N					68.462	13.691	19.178	1.00 23.29 A
	ATOM	699	CA			155		68.012	14.382	17.891	1.00 22.72 A
	ATOM	700	CB			155		66.588	14.916	17.739	1.00 24.25 A
4.5	ATOM	701	CG			155			15.489	16.329	1.00 24.62 A
45	MOTA	702		LEU				66.441	13.798	17.965	1.00 23.10 A
	MOTA	703		LEU				65.576	13.796	19.022	1.00 23.10 A
	ATOM	704	C			155		69.939		19.233	1.00 20.17 A
	ATOM	705	0			155		70.812	14.167 12.088	18.647	1.00 19.72 A
	MOTA	706	N			156		70.227			1.00 13.72 A 1.00 20.11 A
50	MOTA	707	CA			156		71.617	11.693	18.462	1.00 20.11 A
	ATOM	708	CB			156		72.061	10.703	19.540	1.00 20.01 A
	ATOM	709	CG			156.		71.885	11.172	20.963	1.00 20.98 A 1.00 22.18 A
	ATOM	710		TYR				70.619		21.520	1.00 22.18 A 1.00 25.21 A
	MOTA	711		TYR				70.457		22.850	1.00 25.21 A 1.00 21.38 A
55	MOTA	712		TYR				72.991	11.449	21.762	1.00 21.36 A 1.00 25.12 A
	MOTA	713		TYR				72.843	11.859	23.086	1.00 24.83 A
	MOTA	714	CZ			156		71.576	11.995	23.622	1.00 24.03 A 1.00 25.97 A
	MOTA	715	ОН			156		71.431	12.410	24.923	1.00 23.37 A 1.00 20.02 A
	MOVER	716	C	TYR	Α	156		71.792	11.033	17.108	1.00 20.02 A

							•				
	ATOM	717	0	TYR Z	A 15	56	70.959	10.231	16.704	1.00 22.19 A	
	ATOM	718	N	PHE 2	A 19	57	72.860	11.385	16.399	1.00 19.17 A	
	ATOM	719	CA	PHE 2	A 15	57	73.140	10.769	15.114	1.00 18.65 A	
	ATOM	720	CB	PHE I	A 15	57	73.071	11.780	13.969	1.00 21.02 A	
5	ATOM	721	CG	PHE 2	A 15	57	71.719	12.411	13.791	1.00 25.64 A	
	ATOM	722	CD1	PHE 2	A 15	57	70.558	11.724	14.135	1.00 27.84 A	
	MOTA	723		PHE 2			71.603	13.695	13.267	1.00 27.19 A	
	ATOM	724	CE1	PHE 2	A 15	57	69.301	12.310	13.964	1.00 28.87 A	
	ATOM	725	CE2	PHE 2	A 1	57	70.350	14.288	13.091	1.00 28.27 A	
10	MOTA	726	CZ	PHE :	A 15	57	69.200	13.595	13.442	1.00 26.64 A	L
	ATOM	727	C	PHE 2	A 1	57	74.543	10.212	15.204	1.00 19.60 A	L
	ATOM	728	0	PHE .	A 1	57	75.489	10.952	15.467	1.00 19.26 A	k
	ATOM	729	N	GLY .	A 1	58	74.668	8.902	15.010	1.00 19.26 A	k.
	MOTA	730	CA	GLY :	A 1	58	75.972	8.265	15.063	1.00 18.63 A	L
15	ATOM	731	C	GLY .	A 1	58	76.615	8.309	13.693	1.00 16.84 A	L
	ATOM	732	0	GLY .	A 1	58	76.160	7.646	12.772	1.00 15.29 A	L
	MOTA	733	N	LEU .	A 1	59	77.677	9.096	13.567	1.00 18.10 A	k.
	ATOM	734	CA	LEU .	A 1	59	78.386	9.263	12.302	1.00 17.32 A	L
	MOTA	735	CB	LEU .	A 1	59	78.502	10.753	11.984	1.00 16.80 A	L
20	ATOM	736	CG	LEU .	A 1	59	77.161	11.485	12.068	1.00 18.21 A	L
	MOTA	737	CD1	LEU	A 1	59	77.376	12.992	12.058	1.00 15.34 A	¥
	ATOM	738	CD2	LEU .	A 1	59	76.280	11.036	10.906	1.00 14.27 A	Į.
	ATOM	739	С	LEU -	A 1	59	79.780	8.665	12.375	1.00 18.27 A	7
	MOTA	740	0	LEU	A 1	59	80.338	8.518	13.465	1.00 18.92 A	¥
25	ATOM	741	N	SER	A 1	60	80.343	8.320	11.220	1.00 16.88 A	
	MOTA	742	CA	SER	A 1	60	81.691	7.770	11.194	1.00 19.02 A	
	MOTA	743	CB	SER	A 1	60	82.086	7.362	9.771	1.00 20.02 A	
	MOTA	744	OG.	SER	A 1	60	81.866		8.864	1.00 25.88 A	
	ATOM	745	C	SER	A 1	60	82.655		11.724	1.00 18.34 F	
30	MOTA	746	Ο.	SER	A 1	60.	82.413		11.588	1.00 17.84 7	
	ATOM	747	И	TYR	A 1	61	83.743		12.335	1.00 17.11 7	
	MOTA	748	CA	TYR			84.723		12.901	1.00 19.21 F	
	ATOM	749	СВ	TYR			85.146		14.293	1.00 19.37 7	
	MOTA	750	CG	TYR			86.269		14.944	1.00 22.52 F	
35	ATOM	751		TYR			86.276		14.929	1.00 21.17 7	
	MOTA	.752	CE1	TYR			87.283		15.559	1.00 18.10 7	
	MOTA	753	CD2				87.313		15.612	1.00 21.92 7	
	MOTA	754	CE2				88.330		16.252	1.00 20.10 A	
	ATOM	755	CZ	TYR			88.301		16.220	1.00 20.24 7	
40	ATOM	756	он	TYR			89.266		16.873 11.997	1.00 20.31 2	
	ATOM	757	C	TYR			85.934		11.675	1.00 20.13 2	
	ATOM	758	0	TYR			86.623 86.182		11.571	1.00 21.37 2	
	ATOM	759	N	ALA ALA			87.320		10.717	1.00 20.60 2	
45	ATOM	760	CA						9.592	1.00 21.18	
45	ATOM	761	CB	ALA			86.90° 88.37!		11.604	1.00 21.36	
	ATOM	762	C	ALA			88.39		11.752	1.00 20.74	
	ATOM	763	0	ALA LYS			89.23		12.195	1.00 21.80	
	ATOM	764	N CA	LYS			90.29		13.102	1.00 25.38	
50	ATOM	765 766	CB	LYS			91.31		13.332	1.00 30.51	
50	MOTA	767	CG.				90.87		14.251	1.00 38.24	
	ATOM	768	CD	LYS			92.00		14.456	1.00 43.14	
	ATOM	769	CE	LYS			91.55		15.342	1.00 46.63	
	ATOM	770	NZ	LYS			91.25		16.752	1.00 47.21	
55	MOTA MOTA	770	C	LYS			91.08		12.719	1.00 25.07	
J	ATOM	772	0	LYS			91.27			1.00 25.50	
	ATOM	773	и.				91.54		11.477	1.00 25.06	
	ATOM	774	CA	ASN			92.36		11.054	1.00 26.04	
	ATOM	775	CB	ASN			93.11			1.00 26.02	
	ALON										

	MOTA	776	CG	ASN	164	94.062	12.120	10.033	1.00 29.07 A
	MOTA	777	OD1.	ASN A	164	94.854	12.155	10.969	1.00 30.18 A
-	MOTA	778	ND2	ASN A	164	93.979	11.089	9.207	1.00 32.14 A
	MOTA	779	С	ASN A	164	91.725	15.040	10.915	1.00 25.35 A
5	MOTA	780	0	ASN A		92.416	16.021	10.640	1.00 26.51 A
	MOTA	781	N	GLY A	165	90.419	15.122	11.116	1.00 23.92 A
	MOTA	782	CA	GLY A	165	89.761	16.413	11.043	1.00 24.35 A
	MOTA	783	C	GLY A	A 165	89.663	17.123	9.704	1.00 23.94 A
	ATOM	784	0	GLY 3	A 165	89.632	16.501	8.643	1.00 25.49 A
10	MOTA	785	N	GLU A		89.623	18.449	9.773	1.00 23.07 A
	MOTA	786	CA	GLU A	A 166	89.467	19.301	8.602	1.00 23.26 A
	ATOM	787	CB	GLU A	A 166	89.164	20.739	9.036	1.00 23.73 A
	ATOM	788	CG	GLU A	A 166	88.271	20.875	10.257	1.00 27.31 A
	ATOM	789	CD	GLU A	A 166	87.812	22.302	10.474	1.00 29.74 A
15	MOTA	790	OEl	GLU 1	A 166	88.586	23.221	10.130	1.00 30.87 A
	MOTA	791		GLU A	A 166	. 86.686	22.510	10.989	1.00 29.80 A
	MOTA	792	C	GLU		90.612	19.354	7.602	1.00 24.47 A
	ATOM	793	0	GLU I	A 166	91.786	19.473	7.968	1.00 24.85 A
	ATOM	794	N	LEU .	A 167	90.251	19.287	6.328	1.00 23.47 A
20	ATOM	795	CA	PEA 1	A 167	91.228	19.393	5.262	1.00 24.00 A
	MOTA	796	CB,		A 167	90.528	19.369	3.901	1.00 22.48 A
-	MOTA	797	CG	LEU 2	A 167	91.373	19.759	2.679	1.00 23.87 A
	MOTA	798		LEU :		92.583	18.846	2.563	1.00 20.03 A
	MOTA	799	CD2	LEU :		90.516	19.680	1.418	1.00 22.08 A
25	MOTA	800	C		A 167	91.943	20.732		1.00 24.82 A
	MOTA	801	0		A. 167	93.138	20.858	5.165	1.00 24.59 A
	ATOM	802	N		A 168	91.206	21.731	5.927	1.00 24.43 A
	MOTA	803	CA		A 168	91.784	23.055	6.150	1.00 28.25 A
	ATOM	804	CB		A 168	90.746	24.009	6.747	1.00 27.44 A
30	MOTA ·	805	CG		A 168	91.310	25.395	7.090	1.00 28.57 A
,	MOTA	806		LEU		91.624	26.150	5.809	1.00 28.11 A 1.00 29.97 A
	ATOM	807		LEU		90.312	26.174	7.921	1.00 29.97 A 1.00 28.43 A
	ATOM	808	С		A 168	92.999	23.014	7.074	1.00 28.43 A 1.00 30.21 A
	MOTA	809	0		A 168	93.952	23.760	6.882 8.081	1.00 30.21 A
35	ATOM	810	N		A 169	92.958	22.152	9.008	1.00 30.23 A
	MOTA	811	CA		A 169	94.072	22.050	10.046	1.00 35.32 A
	MOTA	812	СВ		A 169	93.821	20.955 20.784	11.033	1.00 33.43 A
	MOTA	813	CG		A 169	94.972	19.562	11.943	1.00 41.43 A
	ATOM	814	CD		A 169	94.808	. 18.261	11.186	1.00 42.67 A
40	ATOM	815	CE		A 169	95.047	17.068	12.096	1.00 43.84 A
	ATOM	816	NZ		A 169	95.329	21.718	8.228	1.00 34.58 A
	ATOM	817	C		A 169 A 169	96.377	22.333	8.421	1.00 35.58 A
	MOTA	818	0		A 170	95.219	20.739	7.339	1.00 34.55 A
4.5	ATOM	819	N			96.357	20.733	6.539	1.00 35.07 A
45	ATOM	820	CA		A 170	96.018	19.047	5.790	1.00 35.72 A
	ATOM	821	CB		A 170	96.050	17.869	6.716	
	ATOM	822	CG		A 170	97.256	17.250	7.040	1.00 39.42 A
	ATOM	823			A 170 A 170	97.313	16.230	7.987	1.00 40.93 A
50	ATOM	824				94.895	17.435	7.355	1.00 38.83 A
50	ATOM .	825	CD2		A 170 A 170	94.937	16.417	8.303	1:00 41.76 A
	ATOM	826	CE2		A 170	96.149	15.821	8.615	1.00 42.18 A
•	ATOM	827 828	OH		A 170	96.196	14.827	9.563	1.00 45.30 A
	ATOM	829	C		A 170	96.823	21.404	5.585	1.00 35.67 A
55	MOTA MOTA	830	0		A 170	97.999	21.465	5.248	1.00 35.28 A
55	ATOM	831	N		A 171	95.904	22.260	5.154	1.00 36.78 A
	ATOM	832	CA		A 171	96.272	23.333	4.252	1.00 38.95 A
	MOTA	. 833	CB		A 171	95.032	24.048	3.682	1.00 39.15 A
	ATOM	834			A 171	95.452	25.329	2.960	1.00 38.11 A

	ATOM	835		ILE			94.296	23.113	2.718	1.00 37.57 A
•	ATOM	836	CD1	IFB	Α	171	93.041	23.712	2.116	1.00 37.48 A
	MOTA	837	C	ILE	Α	171	97.146	24.338	4.990	1.00 41.33 A
	MOTA	838	0	ILE	Α	171	98.173	24.765	4.466	1.00 42.36 A
5	MOTA	839	N	ARG	Α	172	96.748	24.713	6.203	1.00 42.79 A
	ATOM	840	CA	ARG	Α	172	97.541	25.662	6.981	1.00 44.62 A
	ATOM	841	СВ	ARG	Α	172	96.809	26.103	8.253	1.00 46.82 A
	ATOM	842	CG	ARG			95.492	26.828	8.033	1.00 50.73 A
	ATOM	843	CD	ARG			95.124	27.643	9.271	1.00 53.80 A
10	ATOM	844	NE	ARG			93.747	28.136	9.247	1.00 56.88 A
	ATOM	845	CZ	ARG			93.183	28.766	8.218	1.00 57.65 A
	ATOM	846		ARG			93.873	28.989	7.104	1.00 57.71 A
	ATOM	847		ARG			91.923	29.176	8.305	1.00 56.95 A
	ATOM	848	C			172	98.856		7.383	1.00 30.33 A
15								25.015		
13	ATOM	849	0	ARG			99.927	25.587	7.186	1.00 45.16 A
	ATOM	850	N	LYS			98.759	23.817	7.949	1.00 44.01 A
	ATOM	851	CA	LYS			99.923	23.069	8.398	1.00 42.99 A
	ATOM	852	CB	LYS			99.538	21.616	8.667	1.00 44.20 A
00	ATOM	853	CG	LYS			100.721	20.689	8.908	1.00 45.81 A
20	MOTA	854	CD_{\cdot}	LYS			100.272	19.238	8.987	0.00 45.28 A
	ATOM	855	CE	LYS			101.457	18.296	9.120	0.00 45.43 A
•	ATOM	856	NZ	LYS			101.028	16.870	9.146	0.00 45.35 A
	ATOM	857	C	LYS	Α	173	101.081	23.108	7.412	1.00 43.20 A
	MOTA	858	0	LYS	Α	173	102.220	23.366	7.805	1.00 43.49 A
25	MOTA	859	И	ILE			100.802	22.867	6.133	1.00 41.97 A
	MOTA	860	CA	ILE	Ά	174	101.871	22.859	5.136	1.00 40.74 A
	MOTA	861	CB	ILE	Α	174	101.874	21.536	4.336	1.00 40.61 A
	MOTA	862	CG2	ILE	A	174	101.897	20.352	5.297	1.00 41.39 A
	ATOM	863	CG1	ILE	А	174	100.638	21.448	3.442	1.00 40.75 A
30	MOTA	.864	CD1	ILE	Α	174	100.680	20.276	2.487	1.00 40.45 A
	ATOM	865	C	ILE	Α	174	101.882	24.024	4.149	1.00 39.97 A
	ATOM	866	0	ILE	Α	174	102.675	24.033	3.209	1.00 38.15 A
	ATOM	867	N	GLY	Α	175	101.007	25.004	4.359	1.00 40.09 A
	ATOM	868	CA	GLY	Α	175	100.969	26.156	3.473	1.00 39.94 A
35	ATOM	869	C	GLY			100.151	25.960	2.211	1.00 39.87 A
	ATOM	870	0	GLY			99.152	26.646	2.005	1.00 40.53 A
		871	и.	SER			100.586	25.043	1.354	1.00 39.28 A
	ATOM	872	CA	SER			99.871	24.747	0.122	1.00 38.77 A
	ATOM	873	СВ	SER			100.169	25.804	-0.950	1.00 39.84 A
40	ATOM	874	OG	SER			101.537	25.823	-1.319	1.00 43.67 A
	ATOM	875	C	SER			100.265	23.353	-0.358	1.00 38.39 A
	ATOM	876	0	SER			101.245	22.776	0.118	1.00 39.37 A
	ATOM	877	N	PHE			99.491	22.811	-1.289	1.00 35.85 A
	ATOM	878	CA	PHE			99.732	21.472	-1.810	1.00 32.81 A
45					_					1.00 32.30 A
43	ATOM	879	CB CG	PHE			98.401 97.645	20.770	-2.095 -0.867	1.00 32.30 A
		880								1.00 31.20 A 1.00 29.02 A
	ATOM	881		PHE			97.806	21.005	0.348	
	ATOM	882		PHE			96.735	19.293	-0.939	1.00 30.11 A 1.00 27.07 A
50	MOTA	883		PHE			97.076	20.628	1.468	
50	ATOM	884		PHE			95.998	18.910	0.181	1.00 29.70 A
		885	CZ	PHE			96.170	19.580	1.385	1.00 27.57 A
	ATOM	886	C	PHE			100.535	21.485	-3.093	1.00 33.02 A
	ATOM	887	0	PHE			100.386	22.381	-3.927	1.00 30.75 A
	ATOM	888	N	ASP			101.379	20.471	-3.252	1.00 33.87 A
55	ATOM	889	CA	ASP			102.184	20.329	-4.454	1.00 33.45 A
	ATOM	890	CB	ASP			103.269	19.275	-4.244	1.00 35.60 A
	ATOM	891	CG	ASP			102.693	17.932	-3.855	1.00 40.22 A
	MOTA	892		ASP			101.840	17.412	-4.612	1.00 42.64 A
	MOTA	893	OD2	ASP	А	178	103.079	17.398	-2.793	1.00 43.32 A

	ATOM	894		ASP	Α	178		101.195		359	-5.519	1.00	32.	50	A
	ATOM	895				178		99.999	19.7	723	-5.245		30.5		
	ATOM	896				179		101.684	19.5	84	-6.720		31.4		
_	ATOM	897				179		100.790	19.1	160	-7.779		32.0		
5	ATOM	898				179		101.480	19.2	91	-9.138		33.7		
	ATOM	899				179		100.666		11	-10.284		38.8		
	ATOM	900				179		101.129		.95	-11.646		42.7		
	ATOM	901	OB1	GLU	Α	179		102.358	19.3	38	-11.844		43.5		
10	ATOM	902		GLU				100.261		22	-12.523		44.4		
10	ATOM	903	C			179		100.189	17.7	66	-7.635		29.9		
	ATOM	904	0 .			179		99.023			-7.965		27.3		
	ATOM	905	N	THR				100.959	16.8	03	-7.141		30.0		
	ATOM	906	CA	THR				100.429	15.4	48	-7.007		29.7		
15	ATOM	907	CB	THR	A	180		101.583	14.4	16	-6.738		30.6		
15	ATOM	908		THR				101.050	13.2	06	-6.179		30.6		
	ATOM	909	CG2	THR				102.615	14.9	91	-5.802		32.9		
	ATOM	910	C	THR				99.331	15.3	72	-5.935		29.4		
	ATOM	911	0	THR				98.312	14.7	10	-6.130		27.5		
20	ATOM	912	Ŋ	CYS				99.522	16.0	79	-4.823		29.5		
20	ATOM	913	CA	CYS				98.535	16.0	91	-3.745		29.2		
٠.	ATOM	914	CB	CYS	Α	181	•	99.156	16.6	81	-2.480		31.4		
	ATOM	915	SG	CYS				100.580	15.7	47	-1.838		39.8		
	ATOM	916	C	CYS				97.271	16.8	79	-4.126	1.00	28.1	6.	Α
25	ATOM	917	0	CYS				96.156	16.4		-3.762	1.00	26.5	5 2	A
23	ATOM	918	N	THR				97.441	17.9		-4.847		25.7		
	ATOM ATOM	919		THR				96.293	18.7	84	-5.268	1.00	24.2	2 2	A
	ATOM	920	CB	THR				96.714	20.04		-6.066	1.00	24.4	5 2	A
	ATOM	921		THR				97.515	20.9		-5.241		22.5		
30	ATOM	922 923	CG2	THR				95.483	20.80		-6.537		23.43		
50	ATOM	923 924	C	THR .				95.447	17.9		-6.184	1.00	24.7	3 2	A
	ATOM	925	И О	THR .				94.227	17.83		-6.020	1.00	23.72	2 2	A
	ATOM	926		ARG .				96.109	17.28		-7.149	1.00			
	ATOM	927		ARG .				95.422	16.41		-8.096	1.00			
35	ATOM	928		ARG A				96.416	15.78		-9.073	1.00			
	MOTA	929		ARG A				95.740			-10.044	1.00			
	ATOM	930		ARG A				96.704			-11.070	1.00			
	ATOM	931		ARG A				97.260			-11.904	1.00			
	ATOM	932		ARG A				98.502 99.328			11.802	1.00			
40	ATOM	933		ARG A				98.901			10.903	1.00			
•	ATOM	934		ARG A				94.648			12.579	1.00			
•	ATOM	935		ARG A				93.466	15.31		-7.386	1.00			
	ATOM	936		PHE A				95.319	15.09		-7.659	1.00			
	ATOM	937		PHE A				94.689	14.62 13.54		-6.473	1.00			-
45	ATOM	938		PHE A				95.662	12.94		-5,742	1.00			
	ATOM	939		PHE A				95.086	11.78		-4.730	1.00			
	ATOM	940		PHE A				94.958	10.53		-3.961 -4.556	1.00			
	ATOM	941	CD2					94.620	11.96		-4.556	1.00			
	ATOM	942	CE1					94.370	9.46		-3.871	1.00			
50	ATOM	943	CE2	PHE A	. 1	.84	•	94.030	10.90		-1.969	1.00			
	ATOM	944		PHE A				93.904	9.65			1.00			
	ATOM	945		PHE A				93.431	13.97		-2.576 -5.003	1.00			
	ATOM .	946		PHE A				92.353	13.42	, 9	-5.003 -5.219	1.00 2			
•	ATOM	947		CYR A				93.568	14.96		-5.219 -4.124	1.00 2			
55	MOTA	948		ryr a				92.429	15.40		-3.344	1.00 2			
	ATOM	949		CYR A				92.925	16.29		-3.344 -2.200	1.00 2			
	ATOM	950	CG . 3					93.539	15.44		-1.097	1.00 2			
	ATOM	951	CD1 1	YR A	1	85		92.738	14.61		-0.314	1.00 2			
	ATOM	952	CE1 1					93.290	13.73		0.620	1.00 2			

	ATOM	953	CD2	TYR A 185		94.924	15.391	-0.908	28.66	
	MOTA	954	CE2	TYR A 185		95.496	14.514	0.032	29.09 1	
	MOTA	955	CZ	TYR A 185		94.667	13.688	0.790	29.75	
-	MOTA	956	OH	TYR A 185		95.204	12.806	1.702	29.03 2	
5	MOTA	957	С	TYR A 185		91.316	16.058	-4.167	21.02	
	MOTA	958	0	TYR A 185		90.130	15.921	-3.851	18.76	
	MOTA	959	N	THR A 186		91.689	16.731	-5.244	19.87	
	MOTA	960	CA	THR A 186		90.690	17.337	-6.102	18.89	
	MOTA	961	CB	THR A 186		91.344	18.170	-7.200	19.73	
10	MOTA	962	OG1	THR A 186		92.115	19.218	-6.603	19.38	
	MOTA	963	CG2	THR A 186		90.282	18.765	-8.125	20.16	
	MOTA	964	C	THR A 186	i .	89.905	16.201	-6.753	19.05	
	MOTA	965	0	THR A 186	;	88.675	16.244	-6.855	19.38	
	ATOM	966	N	ALA A 187	,	90.627	15.180	-7.200	18.33	
15	MOTA	967	CA	ALA A 187	,	89.984	14.043	-7.841	18.09	
	MOTA	968	CB	ALA A 187		91.024	13.035	-8.276	19.99	
	MOTA	969	C	ALA A 187		88.986	13.402	-6.886	18.07	
	ATOM	970	0	ALA A 187		87.873	13.055	-7.291	18.54	
	ATOM	971	N	GLU A 188	3	89.366	13.253	-5.617	16.56	
20	ATOM	972	CA	GLU A 188	3.	88.446	12.660	-4.653	16.18	
	MOTA	973	CB	GLU A 188	3	89.099	12.495	-3.280	15.52	
	MOTA	974	CG	GLU A 188		90.266	11.519	-3.259	20.99	
`	MOTA	975	CD	GLU A 188		90.297	10.636	-2.013	22.64	
	ATOM	976		GLU A 188		90.006	11.126	-0.899	22.95	
25	MOTA	977		GLU A 188		90.629	9.439	-2.149	27.37	
	ATOM	978	C	GLU A 188		87.189	13.508	-4.518	15.81	
	MOTA	979	0	GLU A 188		86.080	12.978	-4.460	15.92	
	MOTA	980	N	ILE A 189		87.364	14.825	-4.483	16.14	
	MOTA	981	CA	ILE A 189		86.235	15.733	-4.346	16.66	
30	MOTA	982	CB	ILE A 189		86.698	17.179	-4.083	16.57	
	MOTA	983	CG2			85.485	18.098	-3.958	14.92	
	MOTA	984		ILE A 189		87.502	17.235	-2.784	16.19	
:	MOTA	985		ILE A 189		88.202	18.559	-2.547	16.78	
	MOTA	986	С	ILE A 18		85.349	15.712	-5.580	16.29	
35	MOTA	987	0	ILE A 18		84.123	15.667	-5.471	15.80 16.44	
	ATOM	988	N	VAL A 19		85.962	15.743	-6.755	15.98	
	ATOM	989	CA	VAL A 19		85.186	15.704	-7.985	17.23	
	ATOM	990	CB	VAL A 19		86.101	15.692	-9.229	16.01	
_	ATOM	991		VAL A 19		85.280	_	-10.488 -9.373	13.82	
40	ATOM	992		VAL A 19		86.797	17.034	-7.979	16.29	
	MOTA	993	C	VAL A 19		84.351	14.433	-8.194	15.64	
	ATOM	994	0	VAL A 19		83.140	14.462 13.312	-7.723	18.94	
	ATOM	995	N	SER A 19		85.011	12.015	-7.692	18.50	
	ATOM	996	CA	SER A 19		84.337		-7.427	19.04	
45	ATOM	997	CB	SER A 19		85.357	9.680	-7.206	23.87	
	MOTA	998	OG	SER A 19		84.712	11.961	-6.642	16.85	
	ATOM	999	C	SER A 19		83.233	11.281	-6.818	18.11	
	ATOM	1000	0	SER A 19		82.227 83.419	12.671	-5.540	17.37	
	ATOM	1001	N	ALA A 19		82.395	12.687	-4.501	17.10	
50	ATOM	1002	CA	ALA A 19		82.947	13.302	-3.222	17.08	
	ATOM	1003	CB	ALA A 19		81.218		-5.020	18.24	
	ATOM	1004	C	ALA A 19		80.055	13.162	-4.798	18.91	
	MOTA	1005	0	ALA A 19		81.524	14.597	-5.725	16.53	
٠	ATOM	1006	N	LEU A 19		80.483	15.453	-6.270	17.25	
55	ATOM	1007	CA	LEU A 19 LEU A 19		81.091	16.750	-6.826	17.70	
	ATOM	1008	CB			81.537	17.738	-5.732	22.88	
	ATOM	1009	CG.	LEU A 19 L LEU A 19		82.094	19.018	-6.348	22.13	
	ATOM	1010				80.345	18.057	-4.839	20.04	
	MOTA	1011	CD.	2 LEU A 19	J	50.545		• • • • •		

•								•				
	ATOM	1012	C	LEU	A	193	79.664	14.737	-7.343		17.26	
	MOTA	1013	0	LEU	A	193	78.442	14.893	-7.402		15.43	
	ATOM	1014	N	GLU	A	194	80.330	13.962	-8.195	1.00	16.22	A
	ATOM	1015	CA	GLU	Α	194	79.612	13.232	-9.225	1.00	19.22	A.
5	ATOM	1016	CB	GLU	A	194	80.564	12.405	~10.086	1.00	20.77	Α
	ATOM	1017	CG	GLU	Α	194	79.828	11.403	-10.978	1.00	26.27	A
	ATOM	1018	CD	GLU			80.756	10.667	-11.934	1.00	29.43	Α
	ATOM	1019		GLU			81.840		-11.489	1.00	28.21	Α
	MOTA	1020	OE2	GLU			80.392		-13.127	1.00	31.66	Α
10	ATOM	1021	C	GLU			78.599	12.303	-8.566		19.71	
10	ATOM	1021	Ö	GLU			77.466	12.159	-9.027		18.40	
		1022	N	TYR			79.012	11.672	-7.479		19.22	
	ATOM		CA	TYR			78.116	10.773	-6.781		19.69	
	ATOM	1024					78.867	10.041	-5.667		21.39	
	MOTA	1025	CB	TYR			77.975	9.143	-4.847		22.55	
15	MOTA	1026	CG	TYR				7.881	-5.316		23.14	
	MOTA	1027		TYR			77.596				22.98	
	MOTA	1028		TYR			76.743	7.065	-4.577			
	ATOM	1029	CD2	TYR			77.479	9.564	-3.618		21.58	
	MOTA	1030	CE2	TYR			76.625		-2.872		23.50	
20	MOTA	1031	cz	TYR	A,	195	76.263	7.512	-3.358		23.18	
	MOTA	1032	OH	TYR	А	195	75.413	6.732	-2.632		24.19	
	MOTA	1033	С	TYR	А	195	76.939	11.546			18.80	
	ATOM	1034	0	TYR	A.	195	75.782	11.164	-6.337		19.89	
	ATOM	1035	N	LEU	A	196	77.242	12.629	-5.469		15.26	
25	ATOM	1036	CA	LEU	A	196	76.210	13.430	-4.813		16.52	
	ATOM	1037	CB	LEU	Α	196	76.855	14.586	-4.038		15.67	
	MOTA	1038	CG	LEU	Α	196	75.923	15.401	-3.131	1.00	19.13	Α
	ATOM	1039	CD1	LEU	A	196	75.555	14.571	-1.903		18.42	
	ATOM	1040		LEU			76.604	16.681	-2.689	1.00	18.50	Α
30	ATOM	1041	C	LEU	Α	196	75.209	13.993	-5.814	1.00	18.12	Α
-	ATOM	1042	0			196	. 73.990	13.892	-5.637	1.00	16.25	A
	ATOM	1043	N			197	75.732	14.592	-6.875	1.00	17.99	Α
	ATOM	1044	CA			197	74.873	15.171	-7.878	1.00	20.69	Α
	MOTA	1045	СВ			197	75.715	16.004	-8.832	1.00	19.71	A
35	ATOM	1046	CG			197	76.292	17.224		1.00	19.55	Α
رر		1047		HIS			76.069	17.777		1.00	18.32	A
	MOTA	1047		HIS			77.172	18.063		1.00	20.26	Α
	ATOM	1048		HIS			77.463	19.084		1.00	20.73	Α
	ATOM			HIS			76.806	18.935			19.92	
40	ATOM	1050				197	74.091	14.093			22.80	
40	ATOM	1051	C			197	72.974	14.328			21.91	
	MOTA	1052	0			198	74.672	12.903			23.17	
	MOTA	1053	N					11.815	• .		26.22	
	ATOM	1054	CA			198	73.990	11.436			27.16	
	ATOM	1055				198	72.718					_
45	MOTA	1056	0			198	71.837	10.787			27.89 27.84	
	ATOM	1057	N			199	72.623	11.831			28.20	
	MOTA	1058	CA			199	71.429	11.532				
	MOTA	1059	CB			199	71.827	10.952			29.35	
	MOTA	1060	CG			199	72.278				32.74	
50	MOTA	1061	CD			199		8.944			38.22	
	ATOM	1062	CE			199	72.600	7.424			41.17	
	MOTA	1063	NZ			199	73.173	6.779			44.70	
•	MOTA	1064	С			199	70.542	12.765			26.97	
	MOTA	1065	0			199	69.678	12.807			28.27	
55	MOTA	1066	N			200	70.759	13.762			25.62	
	MOTA	1067	CA			200	69.963	14.972			24.75	
	MOTA	1068	С	GLY	Α	200	70.070	15.71			25.82	
	ATOM	1069	0			200	69.080	16.243			26.10	
	МОТА	1070				201	71.275	15.75	-5.353	1.00	25.31	Α

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ATOM 1071 CA ILE A 201 16.440 -4.089 71.490 1.00 26.11 A ATOM 1072 -2.983 CB ILE A 201 71.886 15.438 1.00 27.58 A ATOM 1073 CG2 ILB A 201 72.242 16.175 -1.704 1.00 27.99 A ATOM 1074 CG1 ILE A 201 70.725 14.480 -2.719 1.00 27.89 A ATOM 1075 CD1 ILE A. 201 13.366 -1.746 71.068 1.00 30.62 A -4.233 ATOM 1076 C ILE A 201 72.576 17.489 1.00 25.92 A MOTA 1077 -4.887 O ILE A 201 73.599 17.269 1.00 25.94 A ATOM 1078 N ILE A 202 -3.627 72.337 18.640 1.00 25.04 A ATOM 1079 -3.680 CA ILE A 202 73.289 19.733 1.00 26.57 A 10 ATOM 1080 CB ILE A 202 72.640 20.990 -4.286 1.00 27.69 A CG2 ILE A 202 ATOM 1081 73.695 22.068 -4.516 1.00 30.47 A MOTA 1082 CG1 ILE A 202 -5.625 71.992 20.639 1.00 30.89 A MOTA 1083 CD1 ILE A 202 71.083 21.736 -6.178 1.00 31.79 A ATOM 1084 ILE A 202 73.742 20.032 -2.252 C 1.00 26.14 A 15 ATOM 1085 0 ILE A 202 72.912 20.201 ·-1.351 1.00 24.75 A ATOM 1086 HIS A 203 75.054 -2.042 N 20.075 1.00 25.17 A ATOM 1087 CA HIS A 203 75.585 20.362 -0.717 1.00 24.36 A MOTA 1088 CB HIS A 203 77.095 20.131 -0.677 1.00 23.06 A MOTA 1089 CG HIS A 203 77.680 20.268 0.694 1.00 24.09 A 20 ATOM 1090 CD2 HIS A 203 77.956 21.366 1.434 1.00 22.36 A MOTA 1091 ND1 HIS A 203 77.981 19.183 1.490 1.00 23.65 A MOTA 1092 CE1 HIS A 203 78.418 19.607 2.661 1.00 23.87 A MOTA 1093 NE2 HIS A 203 78.412 20.929 2.653 1.00 25.12 A MOTA 1094 С HIS A 203 75.269 21.811 -0.330 1.00 24.71 A 25 MOTA 1095 0 HIS A 203 74.633 22.055 0.693 1.00 24.27 A MOTA 1096 Ν . ARG A 204 75.724 22.758 -1.154 1.00 25.89 A 75.490 24.199 ATOM 1097 CA ARG A 204 -0.961 1.00 25.68 A ATOM 1098 CB ARG A 204 74.033 24.471 -0.596 1.00 25.57 A MOTA 1099 CG ARG A 204 73.079 24.319 -1.751 1.00 29.26 A 30 ATOM CD . ARG A 204 1100 71.815 25.118 -1.509 1.00 29.86 A ATOM 1101 NE ARG A 204 71.065 24.603 -0.373 1.00 33.90 A 1102 ATOM CZARG A 204 70.021 25.219 0.170 1.00 36.01 A NH1 ARG A 204 ATOM 1103 69.607 26.383 -0.322 1.00 37.08 A ATOM 1104 NH2 ARG A 204 69.387 24.668 1.197 1.00 34.14 A 35 ATOM 1105 C ARG A 204 76.373 24.935 0.034 1.00 26.91 A ATOM 1106 ARG A 204 0 76.210 26.144 0.243 1.00 26.29 A ATOM 1107 N **ASP A 205** 77.303 24.221 0.654 1.00 26.23 A 1108 ASP A 205 ATOM CA 78.203 24.849 1.604 1.00 24.46 A ATOM 1109 CB ASP A 205 24.909 77.557 2.990 1.00 28.25 A 40 ATOM 1110 CG **ASP A 205** 78.203 25.954 3.890 1.00 30.95 A 3.354 ATOM 1111 OD1 ASP A 205 26.862 78.872 1.00 35.13 A OD2 ASP A 205 ATOM 1112 78.034 25.880 5.127 1.00 33.48 A ASP A 205 ATOM 1113 C 79.483 24.039 1.631 1.00 24.22 A 1.00 23.62 A ATOM 1114 0 ASP A 205 79.998 23.676 2.685 45 MOTA LEU A 206 1115 N 79.995 23.755 0.442 1.00 23.31 A LEU A 206 MOTA 1116 CA 81.206 22.978 0.321 1.00 24.19 A LEU A 206 MOTA CB 1117 81.311 22.406 -1.088 1.00 24.78 A MOTA 1118 'CG LEU A 206 82.353 21.309 -1.285 1.00 25.24 A LEU A 206 MOTA 1119. CD1 82.075 20.173 -0.317 1.00 26.72 A 50 MOTA 1120 CD2 LEU A 206 82.298 20.808 -2.720 1.00 24.32 A **LEU A 206** MOTA 1121 C 82.408 23.853 0.623 1.00 24.52 A 1122 **LEU A 206** MOTA ٥ 24.977 82.508 0.130 1.00 24.34 A MOTA 1123 N LYS A 207 23.330 1.424 1.00 22.98 A 83.328 MOTA 1124 CA LYS A 207 24.083 84.517 1.796 1.00 23.05 A 55 LYS A 207 1125 CB 25.305 MOTA 84.113 2.629 1.00 21.18 A CG LYS A 207 24.948 3.830 ATOM 1126 83.278 1.00 19.29 A LYS A 207 MOTA 1127 CD 82.775 26.179 4.568 1.00 23.68 A MOTA 1128 CE LYS A 207 25.781 5.767 1.00 21.99 A 81.913 LYS A 207 26.910 NZMOTA 1129 81.580 6.686 1.00 25.14 A

	A'TTOM	1120	_								11 11 1
	ATOM	1130	C			207	85.44				23.54 A
	ATOM	1131	0			207	85.014				26.04 A
	ATOM	1132	N			208	86.72				23.78 A
_	ATOM	1133	CD			208	87.309		2.100		21.90 A
5	ATOM	1134	CA			208	87.754	22.80			23.64 A
	ATOM	1135	CB	PRO	A	208	88.948	3 23.750	3.397	1.00	22.67 A
	ATOM	1136	CG	PRO	Α	208	88.779	24.432	2.084	1.00	23.00 A
	MOTA	1137	C	PRO	Α	208	87.393	3 22.390	4.859	1.00	24.47 A
	ATOM	1138	0	PRO	Α	208	87.890	21.378	5.358	1.00	24.20 A
10	ATOM	1139	N	GLU	Α	209	86.541	23.176			25.33 A
	ATOM	1140	CA	GLU	Α	209	86.132				26.78 A
	ATOM	1141	CB			209	85.643				27.82 A
	ATOM	1142	CG			209	86.616				34.76 A
	ATOM	1143	CD	GLU			86.459				39.84 A
15	ATOM	1144		GLU			86.575				38.56 A
	ATOM	1145	OE2				86.219				44.97 A
	ATOM	1146	C	GLU			85.039				
	ATOM	1147	Ö	GLU							26.70 A
	ATOM	1148	N	ASN			84.786				29.78 A
20	ATOM						84.395				24.55 A
20		1149	CA	ASN			83.339				24.33 A
	ATOM	1150	CB	ASN			82.195				27.29 A
	ATOM	1151	CG	ASN			81.225			1.00	31.63 A
	ATOM	1152		ASN			80.280				35.25 A
25	ATOM	1153		ASN					6.923	1.00	30.78 A
25	ATOM	1154	С	ASN			83.885			1.00	22.61 A
	ATOM	1155	0	ASN			83.207			1.00	19.95 A
	ATOM	1156	N	ILE			85.105	19.344	4.638	1.00	22.15 A
	MOTA	1157	CA	ILE			85.733	18.174	4.043	1.00	21.36 A
	ATOM	1158	· CB	ILE			86.467	18.538	2.744	1.00	20.33 A
30	MOTA	1159	CG2	ILE			· 87.167	17.315	2.180		20.04 A
	ATOM	1160	CG1	ILE	À.	211	85.475	19.089			19.57 A
	MOTA	1161	CD1	ILE	A	211	86.162	19.718			20.56 A
	MOTA	1162	С	ILE			86.733				22.45 A
	ATOM	1163	0	ILE	Α	211	87.805				21.87 A
35	ATOM	1164	N	LEU			86.377				21.03 A
	ATOM	1165	CA	LEU			87.228				20.43 A
	ATOM	1166	CB	LEU			86.352		7.801		19.57 A
	ATOM	1167	CG	LEU			85.270		8.347		19.01 A
	ATOM	1168	CD1	LEU			84.543		9.494		16.54 A
40	ATOM	1169		LEU			85.903		8.817		19.58 A
	ATOM	1170	C	LEU			88.148		6.139		20.95 A
	ATOM	1171	ō	LEU			88.034		4.983		20.95 A 20.16 A
	ATOM	1172	N	LEU			89.069				
	ATOM	1173	CA	LEU .							21.07 A
45	ATOM	1174		LEU .			89.991	13.330	6.578		21.58 A
	ATOM			LEU .							21.17 A
	ATOM	1176		LEU .			91.633				21.26 A
	ATOM							15.466			23.93 A
		1177		LEU .			91.378		4.070		23.36 A
50	ATOM	1178	C	LEU !			89.912		7.554		22.28 A
50	MOTA	1179	0	LEU .			89.948		8.766		23.80 A
	ATOM	1180	N	ASN A			89.786		7.025		22.96 A
	ATOM	1181		ASN Z			89.718	9.766	7.872	1.00	22.83 A
	ATOM	1182	CB	ASN		214	88.997	8.647	7.103 0	.50 23	.75 AC1
	MOTA	1183	CG	ASN		214	89.144	7.286			.62 AC1
55	ATOM	1184				214	90.212	6.673	7.713 0	.50 25	.34 AC1
	MOTA	1185	ND2			214	88.066	6.803			.41 AC1
	ATOM	1186		ASN A			91.151		8.228		23.68 A
•	ATOM	1187		ASN A			92.112	9.934	7.716		20.85 A
	MOTA	1188	N	GLU A	A :	215	91.291		9.119		

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MOTA 1189 CA **GLU A 215** 92.603 7.901 9.545 1.00 26.20 A MOTA 1190 CB GLU A 215 6.669 10.435 92.453 1.00 26.19 A **ATOM** 1191 CG **GLU A 215** 93.770 6.153 10.985 1.00 29.08 A ATOM 1192 CD. **GLU A 215** 93.589 4.963 11.907 0.00 28.21 A 1193 OE1 GLU A 215 ATOM 93.064 3.927 11.449 0.00 28.42 A ATOM 1194 OE2 GLU A 215 93.973 5.065 13.092 0.00 28.42 A ATOM 1195 С **GLU A 215** 93.532 1.00 26.12 A 7.566 8.385 ATOM 1196 0 GLU A 215 94.746 7.743 8.487 1.00 29.48 A ATOM 1197 N ASP A 216 92.976 7.070 7.287 1.00 25.52 A 10 MOTA 1198 CA **ASP A 216** 93.798 6.728 6.133 1.00 25.79 A CB ASP **ATOM** 1199 216 93.164 5.564 5.376 0.50 27.09 AC1 ATOM 1200 CG ASP 216 93.450 4.231 6.027 0.50 29.11 AC1 ATOM 1201 OD1 ASP 216 93.206 4.098 7.244 0.50 31.09 AC1 ATOM 1202 OD2 ASP 216 93.921 3.315 5.320 0.50 31.52 AC1 15 MOTA 1203 C ASP A 216 1.00 24.88 A 94.034 7.896 5.173 ATOM 1204 O ASP A 216 94.586 7.719 4.094 1.00 26.27 A ATOM 1205 N MET A 217 9.087 5.578 93.615 1.00 25.04 A ATOM 1206 CA MET A 217 93.789 10.301 4.792 1.00 24.86 A ATOM 1207 CB MET A 217 95.270 10.503 4.454 1.00 28.81 A 20 MOTA 1208 CG MET A 217 96.139 10.834 5.676 1.00 29.66 A MET A 217 ATOM 1209 SD 95.577 12.323 6.551 1.00 34.79 A MOTA 1210 CE MET A 217 96.130 13.598 5.411 1.00 30.61 A MOTA 1211 C MET A 217 92.942 10.437 3.528 1.00 24.93 A MOTA 1212 0 MET A 217 93.277 11.215 2.629 1.00 23.08 A 25 ATOM 1213 N HIS A 218 91.855 9.678 3.450 1.00 21.48 A MOTA 1214 CA HIS A 218 90.947 9.799 2.319 1.00 21.72 A ATOM HIS A 218 1215 CB 90.325 8.444 1.963 1.00 21.43 A MOTA 1216 CG HIS A 218 91.225 7.578 1.138 1.00 24.55 A ATOM 1217 CD2 HIS A 218 91.951 6.478 1.458 1.00 23.50 A 30 ATOM ND1 HIS A 218 1218 91.522 7.860 -0.179 1.00 23.64 A MOTA 1219 CE1 HIS A 218 92.392 6.975 -0.633 1.00 21.12 A **ATOM** 1220 NE2 HIS A 218 92.670 6.128 0.340 1.00 22.96 A MOTA 1221 C HIS A 218 89.891 10.785 2.812 1.00 20.49 A MOTA 1222 0 HIS A 218 89.683 10.911 4.018 1.00 20.60 A MOTA 1223 N ILE A 219 89.231 11.488 1.897 1.00 18.82 A MOTA 1224 CA ILE A 219 88.244 12.473 2.306 1.00 17.27 A MOTA 1225 CB ILE A 219 87.914 13.487 1.178 1.00 15.59 A CG2 ILE A 219 MOTA 1226 89.175 14.201 0.718 1.00 14.62 A ATOM CG1 ILE A 219 1227 12.769 87.252 0.006 1.00 16.04 A 40 MOTA 1228 CD1 ILE A 219 86.458 13.685 -0.888 1.00 15.29 A **ATOM** 1229 C ILE A 219 11.885 86.934 2.772 1.00 17.64 A ATOM 1230 0 **ILE A 219** 86.564 10.774 2.402 1.00 18.93 A MOTA 1231 N GLN A 220 86.240 12.658 3.597 1.00 19.19 A ATOM 1232 CA 12.293 **GLN A 220** 84.933 4.119 1.00 21.50 A 45 1233 ATOM CB **GLN A 220** 85.061 11.585 5.475 1.00 23.96 A MOTA 1234 CG **GLN A 220** 85.583 10.151 5.334 1.00 29.77 A **ATOM** 1235 CD **GLN A 220** 84.945 9.182 6.319 1.00 33.77 A OE1 GLN A 220 ATOM 1236 85.257 9.188 7.513 1.00 37.87 A GLN A 220 ATOM 1237 NE2 84.040 8.347 5.821 1.00 34.29 A 50 MOTA 1238 С **GLN A 220** 1.00 21.53 A 84.158 13.599 4.240 MOTA 1239 0 **GLN A 220** 84.367 14.393 5.166 1.00 22.54 A MOTA 1240 N ILE A 221 83.284 13.833 3.270 1.00 19.63 A ATOM 1241 CA 15.054 ILE A 221 82.498 3.234 1.00 19.30 A **ATOM** 1242 CB 15.366 ILE A 221 82.055 1.785 1.00 20.41 A 55 CG2 ILE A 221 MOTA 1243 81.237 16.639 1.738 1.00 19.39 A 15.524 1244 CG1 ILE A 221 ATOM 83.290 0.900 1.00 19.44 A ILE A 221 ATOM 1245 CD1 82.977 15.802 -0.550 1.00 17.44 A С **ATOM** 1246 ILE A 221 81.284 14.951 1.00 18.36 A 4.141 MOTA 1247 0 ILE A 221 80.627 13.911 4.204 1.00 15.98 A

	ATOM	1248	N	THR	Α	222	80.995	16.024	4.864	1.00 19.59 A
	MOTA	1249	CA	THR	А	222	79.844	16.008	5.753	1.00 22.76 A
	ATOM	1250	CB	THR	Α	222	80.218	15.420	7.126	1.00 23.86 A
	MOTA	1251	OG1	THR	Α	222	79.019	15.145	7.863	1.00 28.20 A
5	ATOM	1252	CG2	THR	Α	222	81.105	16.380	7.908	1.00 23.65 A
	ATOM	1253	С	THR	Α	222	79.179	17.370	5.933	1.00 23.55 A
	ATOM	1254	0	THR			79.505	18.334	5.229	1.00 25.65 A
	ATOM	1255	N	ASP			78.248	17.427	6.881	1.00 24.38 A
	ATOM	1256	CA	ASP			77.449.	18.611	7.202	1.00 25.25 A
10	ATOM	1257	CB	ASP			78.303	19.865	7.422	1.00 26.12 A
	ATOM	1258	CG	ASP	А	223	77.538	20.962	8.175	1.00 29.92 A
	ATOM	1259	OD1	ASP	Α	223	76.288	20.876	8.278	1.00 31.91 A
	ATOM	1260	OD2	ASP	А	223	78.177	21.911	8.671	1.00 32.94 A
	ATOM	1261	C	ASP	Α	223	76.461	18.882	6.080	1.00 25.61 A
15	MOTA	1262	0	ASP	Α	223	76.693	19.744	5.227	1.00 25.81 A
	ATOM	1263	N	PHE	A	224	75.358	18.139	6.098	1.00 25.18 A
	ATOM	1264	CA	PHE	A	224	74.310	18.266	5.096	1.00 26.75 A
	MOTA	1265	CB	PHE	Α	224	73.860	16.879	4.635	1.00 27.24 A
	MOTA	1266	CG	PHE	Α	224	74.857	16.189	3.753	1.00 28.10 A
20	ATOM	1267	CD1	PHE	А	224	74.889	16.450	2.388	1.00 29.12 A
	ATOM	1268	CD2	PHE	Α	224	75.790	15.313	4.291	1.00 28.67 A
	MOTA	1269	CE1	PHE	A	224	75.841	15.847	1.567	1.00 30.28 A
	ATOM	1270	CE2	PHE	Α	224	76.745	14.706	3.482	1.00 31.49 A
	ATOM	1271	CZ	PHE	Α	224	76.770	14.973	2.117	1.00 30.54 A
25	ATOM	1272	C .	PHE	Α	224	73.124	19.038	5.632	1.00 27.73 A
	ATOM	1273	0	PHE	A	224	72.005	18.895	5.140	1.00 27.84 A
	ATOM	1274	N	GLY	Α	225	73.378	19862	6.643	1.00 29.36 A
	MOTA	1275	CA	GLY	A	225	72.319	20.656	7.235	1.00 30.10 A
,	MOTA	1276	С	GLY	Α	225	71.825	21.741	6.297	1.00 31.32 A
30	ATOM	1277	0	GLY	Α	225	70.714	22.248	6.451	1.00 32.90 A
	MOTA	1278	N	THR	Α	226	72.640	22.091	5.311	1.00 29.95 A
	MOTA	1279	CA	THR	À	226	72.261	23.132	4.365	1.00 32.06 A
	MOTA	1280	CB	THR	Α	226	73.381	24.167	4.226	1.00 33.35 A
	ATOM	1281	OG1	THR	Α	226	74.454	23.608	3.455	1.00 35.74 A
35	MOTA	1282	CG2	THR	A	226	73.920	24.542	5.593	1.00 34.02 A
	MOTA	1283	C	THR	Α	226	71.979	22.551	2.983	1.00 31.11 A
	ATOM	1284	0	THR	A	226	71.801	23.288	2.012	1.00 30.89 A
	MOTA	12.85	N	ALA	Α	227	71.938	21.230	2.899	1.00 30.02 A
	ATOM	1286	CA	ALA	Α	227	71.714	20.566	1.624	1.00 32.20 A
40	MOTA	1287	CB	ALA	Α	227	71.906	19.057	1.770	1.00 29.19 A
	MOTA	1288	С	ALA	Α	227	70.345	20.865	1.045	1.00 32.77 A
	ATOM	1289	0			227	69.431	21.269	1.761	1.00 34.17 A
	MOTA	1290	N	ALA	Α	228	70.229	20.684	-0.266	1.00 33.18 A
	ATOM	1291	CA	ALA	A	228	68.980	20.902	-0.982	1.00 34.43 A
45	MOTA	1292	CB			228	69.079	22.146		
	ATOM	1293	C			228	68.742	19.674	-1.846	1.00 35.25 A
	MOTA	1294	0			228	69.612	19.284	-2.622	1.00 36.70 A
	MOTA	1295	N			229	67.578	19.056	-1.698	1.00 36.21 A
	ATOM	1296	CA			229	67.246	17.876	-2.488	1.00 37.95 A
50	ATOM	1297	CB			229	66.438	16.857	-1.674	1.00 37.37 A
	ATOM	1298		VAL			66.192	15.609	-2.506	1.00 35.62 A
	MOTA	1299		VAL			67.176	16.522	-0.394	1.00 36.39 A
	MOTA	1300	C			229	66.393	18.341	-3.649	1.00 40.15 A
	MOTA	1301	0			229	65.353	18.965	-3.446	1.00 39.20 A
55	ATOM	1302	N			230	66.836	18.044	-4.865	1.00 43.75 A
	MOTA	1303	CA			230	66.105	18.455	-6.054	1.00 48.04 A 1.00 48.59 A
	ATOM	1304	CB			230	67.039	18.473	-7.258	
	ATOM	1305	CG			230	68.123	19.552	-7.212	1.00 50.35 A
	МОТА	1306	CD1	LEU	Α	230	69.118	19.312	-8.326	1.00 50.62 A

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	MOTA	1307	CD2	LEU	Α	230	67.488	20.932	-7.330	1.00 50.11 A
	MOTA	1308	C	LEU	Α	230	64.905	17.569	-6.346	1.00 51.38 A
	ATOM	1309	0	LEU	A	230	64.929	16.364	-6.095	1.00 51.84 A
	ATOM	1310	N	SER	А	231	63.854	18.190	-6.872	1.00 56.03 A
5	ATOM	1311	·CA	SER			62.616	17.502	-7.224	1.00 60.24 A
	MOTA	1312	CB	SER			61.528	17.806	-6.186	1.00 60.77 A
	MOTA	1313	OG			231	61.222	19.192	-6.150	1.00 61.08 A
	ATOM	1314	C			231	62.115	17.894	-8.622	1.00 62.65 A
	ATOM	1315	ο .	SER			61.527	17.068	-9.326	1.00 63.42 A
10	ATOM	1316	N	PRO			62.334	19.161	-9.040	1.00 64.66 A
	ATOM	1317	CD	PRO			62.903	20.298	-8.289	1.00 64.95 A
	MOTA	1318	CA	PRO			61.882		-10.367	1.00 65.69 A
	ATOM	1319	CB	PRO			62.409		-10.450	1.00 65.77 A
	ATOM	1320	CG	PRO			62.341	21.493	-9.031	1.00 65.77 A
15	ATOM	1321	C	PRO					-11.505	1.00 65.32 A
13	ATOM	1321	0	PRO			62.408			
							62.858		-12.532	1.00 66.55 A
	ATOM	1323	N	ALA			65.927		-3.995	1.00 92.57 A
	ATOM	1324	CA	ALA			67.330	26.100	-3.606	1.00 92.64 A
20	ATOM	1325	CB	ALA			68.187	25.262	-4.558	1.00 92.15 A
20	MOTA	1326	C	ALA			67.769		-3.640	1.00 92.34 A
	ATOM	1327	0	ALA			68.683	27.930	-4.373	1.00 92.47 A
	ATOM	1328	И	ASN			67.108	28.379	-2.833	1.00 91.92 A
	ATOM	1329	CA	ASN			67.396	29.809	-2.767	1.00 91.12 A
	ATOM	1330	CB	ASN			66.374	30.566		1.00 92.32 A
25	ATOM	1331	CG	ASN			64.947	30.084	-3.378	1.00 93.20 A
	MOTA	1332		ASN			64.471	30.061	-2.244	1.00 93.46 A
	ATOM	1333	ND2	ASN			64.261	29.697	-4.452	1.00 94.00 A
	MOTA	1334	C	ASN	А	240	67.334	30.332	-1.335	1.00 89.78 A
	ATOM	1335	. 0	ASN	Α	240	67.766	31.453	-1.053	1.00 89.80 A
30	ATOM	1336	N.	ALA	Α	241	66.787	29.515	-0.441	1.00 88.16 A
	ATOM	1337	CA	ALA	A	241	66.624	29.891	0.955	1.00 86.55 A
	MOTA	1338	С	ALA	А	241	67.901	29.893	1.792	1.00 84.55 A
	ATOM	1339	0	ALA	Α	241	67.865	30.268	2.961	1.00 84.76 A
	MOTA	1340	CB			241	65.583	28.978	1.623	1.00 88.01 A
35	MOTA	1341	N	PHE	Α	242	69.028	29.494	1.216	1.00 82.28 A
	ATOM	1342	CA	PHE	Α	242	70.264	29.483	1.993	1.00 79.83 A
	MOTA	1343	CB	PHE	Α	242	70.718	28.046	2.282	1.00 79.60 A
	ATOM	1344	CG	PHE	Α	242	71.980	27.962	3.100	1.00 79.10 A
	ATOM	1345	CD1	PHE	Α	242	72.024	28.483	4.388	1.00 79.45 A
40	ATOM	1346	CD2	PHE	Α	242	73.131	27.392	2.571	1.00 79.42 A
	ATOM	1347	CE1	PHE	Α	242	73.202	28.442	5.143	1.00 79.29 A
	ATOM	1348	CE2	PHE	A	242	74.314	27.345	3.317	1.00 80.20 A
	MOTA	1349	CZ	PHE	A.	242	74.348	27.872	4.605	1.00 79.98 A
	ATOM	1350.	C	PHE			71.402	30.231	1.322	1.00 77.56 A
45	ATOM	1351.	0	PHE	Α	242	71.347	30.524	0.130	1.00 78.59 A
	ATOM	1352	N	VAL			72.440	30.529	2.098	1.00 73.76 A
	ATOM	1353	CA	VAL			73.595	31.238	1.579	1.00 70.34 A
	MOTA	1354	CB	VAL			73.864	32.515	2.405	1.00 71.71 A
	ATOM	1355		VAL			75.087	33.238	1.859	1.00 71.29 A
50	ATOM	1356		VAL			72.638	33.425	2.376	1.00 71.23 A
	ATOM	1357	C	VAL			74.851	30.362	1.581	1.00 71.41 A
	ATOM	1358		VAL			75.232	29.802	0.552	1.00 66.50 A
	ATOM	1359	И	GLY			75.496	30.245	2.737	1.00 62.34 A
	ATOM	1360	CA	GLY			76.708	29.444	2.737	1.00 62.34 A 1.00 56.48 A
55	ATOM	1361	CA	GLY			77.889	30.327	3.168	1.00 50.48 A 1.00 52.17 A
23	ATOM	1362	0	GLY			77.769	31.547	3.136	1.00 52.17 A 1.00 52.14 A
	ATOM	1363.	И	THR			79.031			1.00 32.14 A
	ATOM	1364	CA	THR			80.201	29.733	3.490	
	ATOM	1365	CB					30.530	3.838	1.00 44.49 A 1.00 45.53 A
	MION	1202	CB	THR	A	245	81.413	29.633	4.106	1.00 45.53 A

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	ATOM	1366	OG1	THR	Α	245	80.994	28.514	4.899	1.00 45.14 A
	MOTA	1367	CG2	THR	Α	245	82.486	30.403	4.873	1.00 42.13 A
	ATOM	1368	C	THR	Α	245	80.523	31.537	2.734	1.00 40.69 A
	ATOM	1369	0	THR	Α	245	80.722	31.175	1.572	1.00 38.45 A
5	ATOM	1370	N	ALA	A	246	80.570	32.804	3.127	1.00 36.53 A
	ATOM	1371	CA	ALA	Α	246	80.816	33.915	2.219	1.00 34.68 A
	ATOM	1372	CB	ALA	Α	246	81.106	35.186	3.023	1.00 34.13 A
	ATOM	1373	C	ALA	А	246 .	81.896	33.718	1.164	1.00 33.21 A
	ATOM	1374	0	ALA	A	246	81.655	33.958	-0.015	1.00 33.62 A
10	ATOM	1375	N	GLN	A		83.082	33.281	1.567	1.00 31.02 A
	ATOM	1376	CA	GLN			84.151	33.112	0.595	1.00 31.05 A
	ATOM	1377	СВ			247	85.476	32.814	1.310	1.00 33.25 A
	ATOM	1378	CG			247	85.921	33.931	2.253	1.00 37.08 A
	ATOM	1379	CD			247	87.378	33.831	2.665	1.00 40.56 A
15	ATOM .	1380		GLN			88.272	34.328	1.972	1.00 41.24 A
	ATOM	1381	NE2			•	87.626	33.180	3.794	1.00 41.86 A
	ATOM	1382	C			247	83.895	32.069	-0.488	1.00 28.53 A
	ATOM	1383	ō	GLN			84.544	32.093	-1.527	1.00 27.93 A
	ATOM	1384	N			248	82.934	31.177	-0.267	1.00 28.01 A
20	ATOM	1385	CA			248	82.643	30.115	-1.238	1.00 28.20 A
. = 0	ATOM	1386	CB	TYR			82.725		-0.532	1.00 24.94 A
	ATOM	1387	CG			248	84.064	28.533	0.126	1.00 23.77 A
	ATOM	.1388		TYR			85.153	28.073	-0.611	1.00 23.01 A
	ATOM	1389	CE1	TYR			86.421	27.975	-0.039	1.00 24.66 A
25	ATOM	1390		TYR			84.270	28.879	1.464	1.00 24.01 A
	ATOM	1391		TYR			85.535	28.785	2.050	1.00 24.49 A
	ATOM	1392	CZ			248	86.606	28.338	1.286	1.00 26.11 A
	ATOM	1393	OH	TYR			87.868	28.305	1.828	1.00 27.54 A
	ATOM	1394	C	TYR			81.301	30.249	-1.961	1.00 28.78 A
30	ATOM	1395	ō	TYR			80.939	29.405	-2.777	1.00 30.26 A
-	ATOM	1396	N	VAL			80.576	31.319	-1.663	1.00 28.83 A
	ATOM	1397	CA	VAL			79.281	31.584	-2.275	1.00 28.70 A
	ATOM	1398	CB	VAL			78.625	32.803	-1.601	1.00 29.37 A
	ATOM	1399		VAL.			77.333	33.163	-2.297	1.00 30.56 A
35	ATOM	1400		VAL			78.376	32.488	-0.127	1.00 31.25 A
0.5	ATOM	1401	C	VAL		•	79.404	31.837	-3.779	1.00 28.19 A
	ATOM	1402	ō	VAL			80.335	32.497	-4.231	1.00 27.69 A
	ATOM	1403	N	SER			78.460	31.308	-4.549	1.00 28.16 A
	ATOM	1404	CA	SER			78.476	31.481	-5.993	1.00 29.05 A
40	ATOM	1405	CB	SER			77.835	30.273	-6.691	1.00 31.08 A
	ATOM	1406	OG			250	76.497	30.058	-6.264	1.00 31.33 A
	ATOM	1407	C	SER			77.737	32.752	-6.376	1.00 29.69 A
	ATOM	1408	ō	SER			76.820	33.191	-5.685	1.00 29.14 A
	ATOM	1409	N	PRO			78.131	33.361	-7.494	1.00 29.35 A
45	ATOM	1410	CD			251	79.147	32.917		1.00 29.28 A
7.5	ATOM	1411	CA	PRO			77.477	34.592	-7.934	1.00 30.27 A
	ATOM	1412	CB	PRO			78.214	34.932	-9.235	1.00 29.87 A
	ATOM	1413	CG	PRO			78.687	33.588	-9.730	1.00 30.48 A
	ATOM .	1414	C	PRO			75.961	34.495	-8.114	1.00 30.86 A
50	ATOM	1415	0	PRO			75.246	35.442	-7.801	1.00 33.28 A
50	ATOM	1416	N	GLU			75.459	33.367	-8.602	1.00 30.19 A
_	ATOM	1417	CA	GLU			74.014	33.244	-8.802	1.00 30.19 A
	ATOM	1417	CB				73.649	31.903	-9.449	1.00 30.51 A
	ATOM	1419	CG	GLU			74.162	30.682	-8.689	1.00 33.88 A
55	MOTA	1419	CD	GLU			75.493	30.882	-9.219	1.00 33.80 A
<i>,,</i>	ATOM	1421		GLU			76.277	30.171	-9.747	1.00 35.25 A
	ATOM	1421		GLU			75.756	28.956	-9.747 -9.095	1.00 33.23 A
	MOTA	1423		GLU			73.750	33.390	-7.494	1.00 32.09 A
	MOTA	1423	0	GLU			72.157	33.928	-7.469	1.00 32.03 A
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	MOTA	1425	N	LEU	Α	253	73.852	32.900	-6.408	1.00 33.87 A
	MOTA	1426	CA	LEU	Α	253	73.230	32.988	~5.096	1.00 35.16 A
	ATOM	1427	CB	LEU	Α	253	74.031	32.183	-4.078	1.00 37.63 A
	ATOM	1428	CG	LEU			73.371	30.937	-3.479	1.00 40.98 A
5	ATOM	1429	CD1	LEU	Α	253	74.302	30.321	-2.433	1.00 42.16 A
	ATOM	1430	CD2	LEU	А	253	72.043	31.314	-2.835	1.00 40.33 A
	ATOM	1431	С	LEU	Α	253	73.148	34.445	-4.640	1.00 37.20 A
	ATOM	1432	0	TEA	А	253	72.300	34.810	-3.820	1.00 37.33 A
	ATOM	1433	N	LEU			74.036	35.276	-5.171	1.00 36.48 A
10	MOTA	1434	CA	LEU			74.052	36.686	-4.816	1.00 37.76 A
	MOTA	1435	CB	LEU	А	254	75.481	37.235	-4.890	1.00 35.47 A
	MOTA	1436	CG	LEU	Α	254	76.512	36.692	-3.899	1.00 32.31 A
	MOTA	1437		LEU			77.839	37.416	-4.108	1.00 32.18 A
	MOTA	1438		LEU	Α	254	76.019	36.891	-2.474	1.00 29.68 A
15	MOTA	1439	C	LEU	Α	254	73.150	37.496	-5.737	1.00 39.82 A
	ATOM	1440	0	LEU	А	254	72.772	38.615	-5.409	1.00 39.15 A
	ATOM	1441	N	THR			72.805	36.919	-6.885	1,00 44.09 A
	ATOM	1442	CA	THR			71.959	37.594	-7.865	1.00 47.95 A
	ATOM	1443	CB	THR			72.591	37.544	-9.276	1.00 48.10 A
20	ATOM	1444	OG1	THR			73.924	38.072	-9.227	1.00 48.96 A
	ATOM	1445	CG2	THR			71.768		-10.253	1.00 50.10 A
•	ATOM	1446	С	THR			70.538	37.032	-7.954	1.00 49.95 A
	MOTA	1447	0	THR			69.631	37.537	-7.300	1.00 51.66 A
	ATOM	1448	N	GLU			70.344	35.994	-8.764	1.00 52.84 A
25	MOTA	1449	CA	GLU		•	69.018	35.395	-8.939	1.00 55.77 A
	ATOM	1450	CB	GLU			69.036		-10.061	1.00 55.24 A
	MOTA	1451	CG	GLU			70.360		-10.790	0.00 55.40 A
	ATOM	1452	CD	GLU			70.699		-11.681	0.00 55.34 A
	ATOM	1453	OE1	GLU			69.831		-12.480	0.00 55.36 A
30	MOTA	1454	OE2	GLU			71.837		-11.593	0.00 55.36 A
	ATOM	1455	C	GLU			68.451	34.743	-7.677	1.00 57.04 A
	ATOM	1456	0			256	67396	34.107	-7.732	1.00 56.82 A
	ATOM	1457	N	LYS			69.137	34.911	-6.549	1.00 58.87 A
25	ATOM	1458	CA	LYS			68.711	34.308	-5.286	1.00 60.38 A 1.00 60.84 A
35	ATOM	1459	CB	LYS			67.607	35.151	-4.623	0.00 60.71 A
	MOTA	1460	CG	LYS			66.327 65.352	35.322 36.261	-5.430 -4.731	0.00 60.71 A
	ATOM	1461	CD	LYS			64.943	35.734	-3.363	0.00 60.77 A
	ATOM	1462	CE NZ	LYS			63.992	36.650	-2.674	0.00 60.77 A
40	ATOM ATOM	1463 1464	C	LYS			68.227	32.878	-5.546	1.00 61.40 A
40	ATOM	1465	0	LYS			67.046	32.565	-5.389	1.00 61.84 A
	ATOM	1466	N.	SER			69.160	32.020	-5.958	1.00 61.26 A
	ATOM	1467	CA	SER			68.865	30.622	-6.271	1.00 61.31 A
	ATOM	1468	CB	SER			68.105	30.548	-7.605	1.00 62.95 A
45	MOTA	1469	OG	SER			68.707	31.374	-8.596	1.00 63.22 A
73	ATOM	1470	C	SER			70.149	29.771	-6.334	1.00 60.39 A
,	ATOM.	1471	0 .	SER			71.257	30.312	-6.329	1.00 60.58 A
	ATOM	1472	N	ALA			70.001	28.447	-6.393	1.00 57.62 A
	ATOM	1473	CA	ALA			71.159	27.551	-6.441	1.00 54.75 A
50	ATOM	1474	CB	ALA			71.670	27.289		1.00 54.90 A
50	ATOM	1475	C	ALA			70.890	26.218	-7.147	1.00 52.13 A
	ATOM	1476	o	ALA			69.759	25.726	-7.175	1.00 51.63 A
	ATOM	1477	И	CYS			71.945	25.641	-7.712	1.00 48.49 A
	ATOM	1478	CA	CYS			71.848	24.371	-8.417	1.00 44.82 A
55	ATOM	1479	CB			260	71.499	24.596	-9.890	1.00 46.78 A
	ATOM	1480	SG	CYS			72.731		-10.821	1.00 53.48 A
	ATOM	1481	C	CYS			73.176	23.643	-8.310	1.00 41.48 A
-	ATOM	1482	ō			260	74.085	24.090	-7.612	1.00 41.05 A
	ATOM	1483	N	LYS			73.288	22.525	-9.012	1.00 37.76 A

	MOTA	1484	CA	LYS	Α	261	74.503	21.729	-8.980	1.00	34.90	A
	MOTA	1485	CB	LYS	Α	261	74.394	20.587	-9.990		35.93	
	ATOM	1486	CG	LYS	Α	261	73.239	19.644	-9.691		38.46	
	MOTA	1487	CD	LYS	А	261 .	73.239	18.430	-10.601		39.70	
5	MOTA	1488	CE	LYS	Α	261	72.117		-10.229		40.95	
	MOTA	1489	NZ	LYS	Α	261	72.076	16.269	-11.110		41.64	
	ATOM	1490	C	LYS	Α	261	75.751	22.556	-9.247		32.19	
	ATOM	1491	0	LYS	A	261	76.780	22.366	-8.595		30.08	
	ATOM	1492	N	SER	Α	262	75.651	23.480	-10.200 .		30.41	
10	MOTA	1493	CA	SER			76.771	24.337	-10.556		27.88	
	MOTA	1494	СВ	SER	Α	262	76./361	25.333	-11.643		29.04	
	ATOM	1495	OG	SER	Α	262	76.398	24.732	-12.921	1.00	32.20	Α
	MOTA	1496	C	SER	Α	262	77.325	25.095	-9.360	1.00	27.01	A
	ATOM	1497	0	SER	Α	262	78.515	25.403	-9.320	1.00	27.37	A
15	ATOM	1498	N	SER	Α	263	76.469	25.406	-8.392	1.00	24.83	Α
	ATOM	1499	CA	SER	Α	263	76.924	26.115	-7.201	1.00	26.29	A
	MOTA	1500	CB	SER	A	2,63	75.758	26.354	-6.242	1.00	26.59	Α
	MOTA	1501	OG	SER	A	263	74.830	27.254	-6.832	1.00	30.68	Α
	MOTA	1502	C	SER	A	263	78.039	25.337	-6.506	1.00	25.15	A
20	ATOM	1503	0	SER	Α	263.	79.034	25.924	-6.078	1.00	25.38	Α
	ATOM	1504	И.	ASP	Α	264	77.884	24.019	-6.396		23.51	
	ATOM	1505	CA	ASP	A	264	78.930	23.215	-5.773	1.00	22.06	A,
	ATOM	1506	CB	ASP	A	264	78.500	21.754	-5.613	1.00	23.87	A
	MOTA	1507	CG	ASP	Α	264	77.378	21.577	-4.599	1.00	27.11	Α
25	ATOM	1508	OD1	ASP	Α	264	77.276	22.402	-3.662	1.00	25.60	A
	ATOM	1509	OD2	ASP	Α	264	76.612	20.599	-4.730	1.00	26.16	Α
	MOTA	1510	С	ASP	Α	264	80.175	23.267	-6.642	1.00	20.62	Α
	ATOM	1511	0	ASP	A	264	81.289	23.339	-6.129	1.00	20.01	A
	MOTA	1512	N	LEU	Α	265	79.985	23.246	-7.959	1.00	18.87	Α
30	ATOM	1513	CA	LEU	Α	265	81.113	23.275	-8.876	1.00	20.02	Α
	ATOM	1514	CB	LEU	A	265	80.634	23.131	-10.322		19.94	
	MOTA	15,15	CG	LEU	Α	265	80.037	21.763	-10.672	1.00	21.08	Α
	MOTA	1516	CD1	LEU	Α	265	79.580	21.771	-12.122	1.00	22.16	A
	ATOM	1517	CD2	LEU	Α	265	81.077	20.659	-10.449	1.00	16.76	A
35	ATOM	1518	С	LEU	Α	265	81.910	24.552	-8.705	1.00	20.53	A
	ATOM	1519	0	LEU	Α	265	83.130	24.563	-8.881	1.00	21.94	Α
	ATOM	1520	N	TRP	Α	266	81.221	25.633	-8.361	1.00	21.74	Α
	ATOM	1521	CA	TRP	Α	266	81.897	26.899	-8.138	1.00	20.89	A
•	ATOM	1522	CB	TRP	Α	266	80.879	28.031	-7960	1.00	22.97	A
40	ATOM	1523	CG	TRP	Α	266	81.477	29.309	-7.411	1.00	24.01	Α
	ATOM	1524	CD2	TRP	Α	266	81.814	30.487	-8.152	1.00	23.31	Α
	ATOM	1525	CE2	TRP	Α	266	82.391	31.404	-7.243	1.00	23.27	Α
	MOTA	1526	CE3	TRP	Α	266	81.689	30.858	-9.497	1.00	24.79	A
	ATOM	1527	CD1	TRP			81.850	29.555	-6.116		24.55	
45	MOTA	1528	NE1	TRP	Α	266	82.401	30.811	-6.009	1.00	23.65	Α
	ATOM	1529		TRP			82.839	32.663	-7.636	1.00	22.89	Α
	ATOM	1530	CZ3				82.139	32.116	-9.887	1.00	23.30	Α
•	ATOM	1531	CH2		Α	266	82.705	33.000	-8.959	1.00	23.32	A
	ATOM	1532	C		Α	266	82.739	26.735	-6.877	1.00	20.30	Α
50	ATOM	1533	Ō			266	83.913	27.102	-6.853	1.00	20.60	Α
	ATOM	1534	N			267	82.141	26.175	-5.832	1.00	18.06	A
	ATOM	1535	CA			267	82.868	25.966	-4.584	1.00	18.46	A
	MOTA	1536	СВ			267	81.984	25.254	-3.561	1.00	17.96	Α
	MOTA	1537	C			267	84.112	25.132	-4.877	1.00	18.05	A
55	ATOM	1538	0			267	85.173	25.340	-4.287	1.00	17.35	A
	ATOM	1539	N			268	83.982	24.190	-5.799		17.12	
	ATOM	1540	CA			268	85.118	23.355	-6.157	1.00	18.45	Α
	MOTA	1541	СВ			268	84.703	22.326	-7.204		17.67	
	ATOM	1542	CG			268	85.809	21.436	-7.772	1.00	16.93	A
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MOTA 1543 CD1 LEU A 268 86.333 20.495 -6.704 1.00 17.10 A 1544 20.651 ~8.953 ATOM CD2 LEU A 268 1.00 13.46 A 85.258 ATOM 1545 С **LEU A 268** 24.249 -6.705 1.00 19.64 A 86.232 ATOM 1546 0 **LEU A 268** 87.389 24.129 -6.306 1.00 18.99 A ATOM 1547 N **GLY A 269** 85.869 25.158 -7.606 1.00 19.16 A 26.057 1.00 18.25 A 1548 **GLY A 269** -8.178 ATOM CA 86.854 ATOM 1549 C **GLY A 269** 26.804 -7.103 1.00 20.30 A 87.604 MOTA 1550 0 **GLY A 269** 88.825 26.960 -7.178 1.00 20.24 A 1.00 20.20 A 1551 27.266 -6.090 ATOM N CYS A 270 86.874 10 ATOM 1552 CA CYS A 270 87.486 27.996 -4.986 1.00 20.73 A -4.031 CB 28.523 ATOM 1553 CYS A 270 86.418 1.00 21.05 A CYS A 270 29.703 -4.752 1.00 23.98 A MOTA 1554 SG 85.292 MOTA 1555 С CYS A 270 88.417 27.082 -4.206 1.00 20.77 A 1556 CYS A 270 89.550 27.449 -3.878 1.00 22.00 A ATOM 0 15 ATOM 1557 N ILE A 271 87.927 25.886 -3.907 1.00 19.32 A 1558 88.704 24.921 -3.147 1.00 18.46 A ATOM CA ILE A 271 23.668 -2.861 1.00 15.71 A MOTA 1559 CB ILE A 271 87.872 22.607 ATOM 1560 CG2 ILE A 271 88.722 -2.182 1.00 16.51 A 1561 CG1 ILE A 271 86.688 24.051 -1.974 1.00 14.97 A MOTA 1.00 17.80 A 20 CD1 ILE A 271 85.785 22.891 -1.639 MOTA 1562 С 90.001 24.546 -3.856 1.00 19.30 A MOTA 1563 ILE A 271 ILE A 271 1564 91.062 24.532 -3.242 1.00 21.30 A MOTA O 1.00 20.07 A MOTA 1565 N ILE A 272 89.915 24.253 -5.147 CA 1566 ILE A 272 91.094 23.894 -5.906 1.00 21.50 A ATOM 25 ILE A 272 23.693 -7.385 1.00 22.57 A MOTA 1567 CB 90.758 1.00 21.91 A ILE A 272 92.041 23.498 -8.184 MOTA 1568 CG2 1.00 23.57 A ATOM 1569 CG1 ILE A 272 89.818 22.495 -7.542 CD1 ILE A 272 89.314 22.294 -8.949 1.00 24.20 A ATOM 1570 1.00 22.90 A -5.794 ILE A 272 25.010 ATOM 1571 C 92.112 30 24.783 -5.507 1.00 21.82 A 1572 ILE A 272 93.287 ATOM O ATOM 1573 N **TYR A 273** 91.638 26.226 -6.028 1.00 24.81 A ATOM 1574 CA TYR A 273 92.478 27.400 -5.969 1.00 25.15 A 1.00 26.04 A -6.255 ATOM 1575 CB TYR A 273 91.630 28.632 **TYR A 273** 92.385 29.931 -6.173 1.00 27.80 A ATOM 1576 CG 92.715 30.500 -4.939 1.00 27.53 A 35 1577 **TYR A 273** ATOM CD1 -4.870 1.00 27.30 A 1578 CE1 **TYR A 273** 93.405 31.708 ATOM ATOM 1579 CD2 TYR A 273 92.765 30.602 -7.333 1.00 27.17 A ATOM 1580 CE2 **TYR A 273** 93.448 31.804 -7.277 1.00 26.68 A TYR A 273 93.766 32.355 -6.050 1.00 28.05 A CZMOTA 1581 40 MOTA 1582 OH **TYR A 273** 94.433 33.562 -6.018 1.00 30.80 A TYR A 273 27.521 -4.599 1.00 26.05 A MOTA 1583 C .93.139 MOTA 1584 **TYR A 273** 94.310 27.889 -4.489 1.00 24.45 A 0 -3.556 ATOM 1585 N **GLN A 274** 92.380 27.205 1.00 25.95 A **GLN A 274** 92.896 27.299 -2.202 1.00 25.98 A ATOM 1586 CA 27.209 -1.199 1.00 25.56 A MOTA CB **GLN A 274** 91.743 1587 MOTA 1588 CG **GLN A 274** 92.169 27.422 0.233 1.00 25.42 A **GLN A 274** 90.990 27.571 1.161 1.00 28.69 A ATOM 1589 CD OE1 **GLN A 274** 89.838 27.506 0.732 1.00 29.84 A ATOM 1590 ATOM 1591 NE2 **GLN A 274** 91.267 27.774 2.445 1.00 29.83 A 50 **GLN A 274** 26.231 -1.915 1.00 25.08 A MOTA 1592 C 93.951 26.452 -1.120 **GLN A 274** 94.862 1.00 24.38 A ATOM 1593 0 1.00 24.42 A -2.567 25.081 MOTA 1594 N **LEU A 275** 93.838 **LEU A 275** 24.006 -2.369 1.00 25.43 A 94.813 MOTA 1595 CA **LEU A 275** 22.713 -3.035 1.00 22.95 A MOTA 1596 CB 94.335 1.00 25.67 A -2.354 55 MOTA 1597 CG LEU A 275 93.193 21.959 LEU A 275 1.00 22.16 A CD1 20.702 -3.154 92.817 MOTA 1598 1599 CD2 LEU A 275 93.633 21.580 -0.950 1.00 23.32 A MOTA **LEU A 275** -2.948 1.00 25.40 A 1600 C 96.171 24.376 MOTA 1.00 25.87 A -2.376 MOTA 1601 0 LEU A 275 97.212 24.071

1.00 25.78 A 25.039 -4.094 **VAL A 276** 96.153 MOTA 1602 N 1.00 26.12 A **VAL A 276** 25.419 -4.759 MOTA 1603 CA 97.384 1.00 26.14 A VAL A 276 97.170 25.522 -6.280 MOTA 1604 CB -6.962 1.00 24.46 A 25.783 ATOM 1605 CG1 VAL A 276 98.492 1.00 22.55 A -6.804 VAL A 276 24.248 MOTA 1606 CG2 96.531 VAL A 276 26.735 -4.275 1.00 27.83 A 97.990 C MOTA 1607 1.00 29.55 A 1608 26.849 -4.164 0 VAL A 276 99.210 MOTA 1.00 26.88 A -3.990 ALA A 277 97.148 27.723 1609 N MOTA 29.023 -3.549 1.00 26.50 A CA АLA A 277 97.639 MOTA 1610 1.00 24.49 A ALA A 277 30.126 -4.122 10 MOTA 1611 CB 96.765 -2.035 1.00 26.79 ALA A 277 97.740 29.175 C ATOM 1612 1.00 28.26 30.042 -1.548 0 ALA A 277 98.465 ATOM 1613 1.00 26.17 A -1.290 MOTA 1614 N **GLY A 278** 97.020 28.343 1.00 24.63 A 0.159 97.074 28.430 CA **GLY A 278** ATOM 1615 1.00 25.52 A **GLY A 278** 29.272 0.780 95.971 15 MOTA 1616 С **GLY A 278** 1.998 1.00 27.25 A 1617 0 95.793 29.259 ATOM 1.00 24.94 A 29.998 -0.051 1618 **LEU A 279** 95.229 ATOM N 0.408 1.00 25.58 A 94.130 30.849 1619 CA **LEU A 279** ATOM 0.522 1.00 27.65 A CB **LEU A 279** 94.603 32.302 ATOM 1620 32.631 1.470 1.00 29.35 A 95.748 LEU A 279 20 MOTA 1621 CG 96.365 1.075 1.00 30.47 A LEU A 279 33.958 1622 CD1 MOTA 1.00 29.70 A CD2 LEU A 279 95.232 32.671 2.892 ATOM 1623 1.00 25.19 A -0.605 **LEU A 279** 92.987 30.822 ATOM 1624 C 30.525 -1.781 1.00 25.34 A 1625 0 **LEU A 279** 93.201 ATOM 1.00 23.60 A 91.755 31.126 -0.165 PRO A 280 25 MOTA 1626 N 91.306 31.357 1.216 1.00 22.97 A ,CD PRO A 280 MOTA 1627 1.00 23.81 A -1.103 PRO A 280 90.628 31.133 MOTA 1628 CA -0.195 1.00 25.19 A PRO A 280 89.417 31.338 MOTA 1629 CB 1.00 25.48 A 32.041 1.008 89.982 ATOM 1630 CG PRO A 280 PRO A 280 90.855 32.295 -2.083 1.00 26.26 30 C MOTA 1631 33.207 -1.792 1.00 25.42 A MOTA 0 PRO A 280 91.632 1632 -3.243 1.00 26.49 A 32.284 MOTA 1633 N PRO A 281 90.178 31.285 -3.651 1.00 27.13 A 89.182 MOTA 1634 CD PRO A 281 1.00 27.25 A 33.316 -4.281 PRO A 281 90.307 ATOM 1635 CA 32.727 -5.463 1.00 26.75 A 89.522 PRO A 281 35 ATOM 1636 CB 1.00 25.29 A 89.354 31.291 -5.136 CG PRO A 281 1637 MOTA 1.00 27.30 A -3.954 MOTA 1638 C PRO A 281 89.817 34.724 35.709 -4.238 1.00 27.67 A 90.497 1639 0 PRO A 281 ATOM 88.623 34.817 -3.388 1.00 27.79 A PHE A 282 MOTA 1640 N 36.107 -3.066 1.00 28.37 A 40 1641 CA PHE A 282 88.034 ATOM 1.00 27.77 A -3.467 86.563 36.086 1642 CB PHE A 282 MOTA 35.557 -4.857 1.00 29.06 A 1643 PHE A 282 86.335 ATOM CG -5.965 1.00 28.74 A 36.392 ATOM 1644 CD1 PHE A 282 86.454 34.207 -5.063 1.00 25.80 A 86.077 1645 CD2 PHE A 282 MOTA 86.324 35.887 -7.255 1.00 28.50 A 1646 CE1 PHE A 282 45 ATOM 33.695 -6.346 1.00 26.04 A **MOTA** 1647 CE2 PHE A 282 85.947 34.535 -7.444 1.00 28.02 A 86.071 1648 CZPHE A 282 MOTA 88.184 36.426 -1.589 1.00 29.95 A C PHE A 282 MOTA 1649 -0.741 1.00 32.95 A ATOM 1650 O PHE A 282 87.600 35.763 1.00 32.36 A 88.977 37.445 -1.285 50 1651 N ARG A 283 ATOM 37.843 0.100 1.00 33.06 A CA ARG A 283 89.215 ATOM 1652 37.432 0.520 1.00 33.69 A MOTA 1653 CB ARG A 283 90.622 90.990 36.006 0.151 1.00 36.29 A ARG A 283 1654 CG MOTA 1.00 38.81 A 35.635 0.727 1655 CD ARG A 283 92.341 MOTA 0.133 1.00 41.73 A 36.423 55 ATOM 1656 NE ARG A 283 93.415 36.338 -1.142 1.00 44.14 A 93.783 CZ1657 ARG A 283 MOTA -1.958 1.00 45.19 A NH1 ARG A 283 93.162 35.497 1658 MOTA 1.00 44.57 A 94.772 37.094 -1.604 1659 NH2 ARG A 283 MOTA 39.353 1.00 32.44 A 1660 ARG A 283 0.267 MOTA С 89.065

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	MOTA	1661	0	ARG	A	283		89.429	40.118	-0.624		31.91	
	MOTA	1662	N	ALA	Α	284		88.527	39.777	1.406		33.21	
	MOTA	1663	CA	ALA	A	284		88.348	41.199	1.682		32.82	
	ATOM	1664	CB	ALA	Α	284		87.265	41.777	0.782		32.40	
5	MOTA	1665	С	ALA	Α	284		88.004	41.445	3.147		32.98	
•	ATOM	1666	0	ALA				87.779	40.502	3.913		32.53	
	MOTA	1667	N	GLY				87.961	42.723	3.520		32.60	
	MOTA	1668	CA	GLY				87.666	43.112	4.887		30.00	
	MOTA	1669	С	GLY	Α	285		86.355	42.637	5.486	-	29.37	
10	MOTA	1670	0	GLY	A	285		86.287	42.366	6.685		29.35	
	ATOM	1671	N	ASN				85.302	42.547	4.685		28.99	
	MOTA	1672	CA	ASN	Α	286		84.024	42.097	5.226		29.58	
	MOTA	1673	CB	ASN	Α	286		83.238	43.281	5.801		29.54	
	MOTA	1674	CG	ASN			•	82.958	44.356	4.764		29.60	
15	ATOM	1675		ASN				82.350	44.092	3.720		26.48	
	MOTA	1676	ND2	ASN				83.400	45.575	5.049		25.96	
	MOTA	1677	C	ASN	А	286		83.196	41.378	4.182		30.16	
	MOTA	1678	0	ASN	Α	286		83.551	41.357	3.004		31.70	
	MOTA	1679	\mathbf{N}	GLU	Α	287		82.084	40.796	4.613		31.14	
20	MOTA	1680	CA	GLU	A	287		81.225	40.051	3.699		32.53	
	MOTA	1681	CB	GLU	Α	287		79.943	39.600	4.397		35.66	
	ATOM	1682	CG	GLU	Α	287		80.168	38.813	5.666	-	43.05	
	MOTA	1683	CD	GLU	Α	287		79.138	37.707	5.856		47.79	
	MOTA	1684	OE1	GLU	A	287		77.933	37.959	5.616		49.01	
25	ATOM	1685	OE2	GLÜ	Α	287		79.539	36.588	6.256		48.82	
	ATOM	1686	С	GLU	Α	287		80.853	40.837	2.457		30.19	
	ATOM	1687	0	GLU	A	287		80.986	40.332	1.343		30.33	
	ATOM	1688	N	TYR	A	288		80.385	42.066	2.653		29.13	
	ATOM	1689	CA	TYR	Α	288		79.972	42.922	1.541		27.98	
30	MOTA	1690	CB	TYR	Α	288		79.573	44.320	2.034		26.59	
	ATOM	.1691	CG	TYR	A	288		79.080	45.217	0.917		26.43	
•	ATOM	1692	CD1	TYR	A	288		77.799	45.060	0.385		28.06	
	MOTA	1693	CE1	TYR	Α	288		77.350	45.854	-0.675		28.72	
	MOTA	1694	CD2	TYR	A	288		79.905	46.196	0.363		27.24	
35	MOTA	1695	CE2	TYR	A	288		79.470	46.994	-0.697		28.55	
	MOTA	1696	CZ	TYR	Α	288		78.192	46.814	-1.211		29.91	
	MOTA	1697	ОН	TYR	А	288		77.765	47.571	-2.275		30.53	
	MOTA	1698	C	TYR	A	288		81.057	43.068	0.487		25.84	
	MOTA	1699	0	TYR	Α	288		80.790	42.940	-0.701		27.88	
40	MOTA	1700	И	LEU	Α	289		82.279	43.344	0.919		24.24	
	ATOM	1701	CA	LEU	A	289		83.382	43.495	-0.018		26.60	
	ATOM	1702	CB	LEU	Α	289		84.662	43.919	0.713		25.15	
	MOTA	1703	CG	LEU	`A	289		85.005	45.411	0.817		27.82	
	MOTA	1704	CD1	LEU	Α	289		83.830	46.277	0.354		27.32	
45	MOTA	1705	CD2	LEU	Α	289		85.404	45.727	2.251		25.62	
	ATOM	1706	С	LEU	A	289		83.622	42.184	-0.736		27.45	
	ATOM	1707	0	LEU	Α	289		83.901	42.157	-1.933		30.18	
	MOTA	1708	N	ILE	Α	290		83.520	41.093	0.009		28.11	
	ATOM	1709	CA			290		83.726	39.770	-0.551		28.84	
50	MOTA	1710	CB	ILE	Α	290		83.565	38.710	0.545		29.67	
	ATOM	1711	CG2					83.450	37.331	-0.071		31.47	
	MOTA	1712	CG1	ILE	A	290		84.756	38.802	1.504		29.26	
	MOTA	1713	CD1	ILE	A	290		84.604	37.995	2.779		27.48	
	MOTA	1714	C			290		82.727	39.530	-1.676		27.99	
55	MOTA	1715	0	ILE	Α	290		83.090	39.110	-2.775		26.63	
	MOTA	1716	· N			291		81.464	39.824	-1.406		28.54	
	MOTA	1717	CA			291		80.432	39.638	-2.407		27.14	
	MOTA	1718	CB			291		79.066	39.945	-1.807		28.37	
	MOTA	1719	CG	PHE	Α	291		78.674	39.024	-0.688	1.00	30.37	, A

	MOTA	1720	CD1	PHE	A	291		79.283	37.778	-0.543	1.00 30.07 A
	MOTA	1721	CD2	PHE	Α	291		77.658	39.377	0.194	1.00 29.74 A
	MOTA	1722	CE1	PHE	Α	291		78.885	36.897	0.463	1.00 32.11 A
	MOTA	1723	CE2	PHE	Α	291		77.253	38.502	1.202	1.00 32.76 A
5	MOTA	1724	CZ	PHE	A	291		77.867	37.259	1.336	1.00 32.01 A
	MOTA	1725	C	PHE	Α	291		80.690	40.525	-3.618	1.00 27.79 A
	MOTA	1726	0	PHE	Α	291		80.434	40.124	-4.755	1.00 26.52 A
	MOTA	1727	N	GLN	A	292		81.200	41.730	-3.384	1.00 27.05 A
	MOTA	1728	CA	GLN	Α	292		81.478	42.613	-4.503	1.00 27.48 A
10	MOTA	1729	CB	GLN	Α	292		82.072	43.945	-4.037	1.00 27.80 A
	MOTA	1730	CG	GLN	Α	292		81.041	44.984	-3.651	1.00 30.50 A
	ATOM	1731	CD	GLN			•	81.630	46.381	-3.565	1.00 31.30 A
	ATOM	1732	OE1	GLN	А	292		82.519	46.644	-2.762	1.00 33.17 A
•	MOTA	1733	NE2	GLN	А	292		81.133	47.284	-4.399	1.00 32.86 A
15	ATOM -		C	GLN				82.442	41.934	-5.460	1.00 26.82 A
	MOTA	1735	ō	GLN				82.186	41.883	-6.664	1.00 28.03 A
	MOTA	1736	N	LYS				83.539	41.402	-4.924	1.00 24.08 A
	MOTA	1737	CA	LYS				84.542	40.739	-5.751	1.00 24.43 A
	ATOM	1738	CB	LYS			•	85.752	40.368	-4.901	1.00 26.19 A
20	MOTA	1739	CG	LYS				86.456	41.580	-4.319	1.00 28.24 A
20	ATOM	1740	CD	LYS				87.750	41.213	-3.608	1.00 30.60 A
	ATOM	1741	CE	LYS				88.555	42.468	-3.273	1.00 32.23 A
	ATOM	1742	NZ	LYS				89.849	42.170	-2.591	1.00 32.86 A
	ATOM	1742	C	LYS				84.008	39.500	-6.472	1.00 25.06 A
25	ATOM	1744	0	LYS				84.350	39.236	-7.628	1.00 24.96 A
23	MOTA	1745	N .	ILE				83.163	38.740	-5.793	1.00 24.33 A
	ATOM	1746	CA	ILE				82.593	37.552	-6.399	1.00 24.46 A
	ATOM	1747	ĊB	ILE				81.725	36.800	-5.385	1.00 22.52 A
	ATOM	1748	CG2	ILE				80.837	35.783	-6.093	1.00 23.14 A
30	ATOM	1749	CG1	ILE				82.632	36.141	-4.345	1.00 21.54 A
50	ATOM	1750	CD1			-		81.892	35.535	-3.175	1.00 19.38 A
	ATOM	1751	C			294		81.761	37.885	-7.639	1.00 27.01 A
	ATOM	1752	0			294		81.967	37.303	-8.704	1.00 23.93 A
	ATOM	1753	И			295		80.830	38.828	-7.513	1.00 29.79 A
35	ATOM	1754	CA	ILE				79.983	39.168	-8.653	1.00 32.98 A
55	ATOM	1755	CB			295		78.767	40.004	-8.228	1.00 33.96 A
	ATOM	1756	CG2	ILE				77.980	39.246	-7.174	1.00 36.23 A
	ATOM	1757	CG1	ILE				79.216	41.358	-7.682	1.00 35.79 A
	ATOM	1758	CD1					78.062	42.266	-7.300	1.00 37.79 A
40	ATOM	1759	C			295		80.729	39.898	-9.757	1.00 33.17 A
40 .	ATOM	1760	o			295		80.212		-10.862	1.00 34.06 A
	ATOM	1761	N	•		296		81.946		9.462	1.00 33.65 A
	ATOM	1762	CA			296		82.747		-10.468	1.00 34.81 A
		1763	CB			296		83.353		-9.895	1.00 38.05 A
45	ATOM	1764				296		82.353	43.427	-9.714	1.00 40.12 A
43	ATOM	1765	CD			296		83.070	44.736	-9.401	1.00 44.01 A
	MOTA	1766	CE			296		82.191	45.939	-9.731	1.00 46.66 A
	MOTA	1767	NZ			296		82.972	47.209	-9.833	1.00 47.40 A
	MOTA	1768	C			296		83.851		-10.945	1.00 34.15 A
50	ATOM	1769	0			296		84.622	-	-11.847	1.00 33.48 A
30	ATOM					297		83.907		-10.333	1.00 33.82 A
	ATOM	1770	N CA	FEO				84.904		-10.555	1.00 33.02 A
	ATOM	1771	CB					84.716		-12.110	1.00 32.00 A
	MOTA	1772	CB			297 297		85.452		-12.110	1.00 32.43 A 1.00 33.09 A
55	ATOM	1773		PEA				84.959		-12.536	1.00 31.88 A
55	MOTA	1774		LEU				85.206		-14.025	1.00 31.00 A 1.00 32.51 A
	MOTA	1775				297 297		86.275		-10.476	1.00 32.31 A
	MOTA	1776	C			297 297		87.180		-11.278	1.00 32.23 A
	ATOM	1777 1778	И О			297 298		86.424	39.267	-9.395	1.00 32.00 A 1.00 33.56 A
•	MOTA	T / / Q	14	GTIO	А	230		30.444	22.201	-9.393	

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39.936 -9.110 1.00 35.66 A 1779 **GLU A 298** 87.682 MOTA CA 87.405 1.00 38.03 A **GLU A 298** 41.274 -8.428 1780 CB ATOM **GLU A 298** 42.125 -8.236 1.00 42.97 A MOTA 1781 CG 88.641 1.00 46.19 A MOTA 1782 CD **GLU A 298** 88.383 43.313 -7.338 1.00 48.41 A -7.602 ATOM 1783 OE1 GLU A 298 87.412 44.055 43.504 -6.369 1.00 48.44 A OE2 GLU A 298 89.153 MOTA 1784 -8.245 1.00 34.35 A 1785 C **GLU A 298** 88.644 39.117 MOTA 1.00 35.64 A **GLU A 298** 39.065 -7.021 1786 0 88.508 MOTA -8.894 38.478 1.00 32.46 A TYR. A 299 89.611 MOTA 1787 Ν -8.208 1.00 30.71 A 10 MOTA 1788 CA TYR A 299 90.624 37.678 1.00 26.01 A TYR A 299 90.031 36.367 -7.672 CB MOTA 1789 35.300 -8.730 1.00 26.77 A CG TYR A 299 89.874 1790 MOTA 1.00 26.60 A -9.699 MOTA 1791 CD1 TYR A 299 88.871 35.390 -10.724 1.00 26.10 A 34.448 CE1 TYR A 299 88.768 MOTA 1792 34.236 -8.807 1.00 22.56 A TYR A 299 90.770 15 MOTA 1793 CD2 -9.822 1.00 24.59 A 1794 CE2 TYR A 299 90.677 33.291 MOTA 1.00 26.34 A 89.674 33.400 -10.781 TYR A 299 MOTA 1795 CZ 32.463 -11.791 1.00 22.44 A TYR A 299 89.578 1796 OH ATOM 1.00 30.95 A -9.229 1797 **TYR A 299** 91.720 37.374 MOTA C 37.575 -10.425 1.00 28.80 A 20 TYR A 299 91.528 MOTA 1798 0 -8.764 1.00 33.38 A **ASP A 300** 92.865 36.891 1799 N **ATOM** 1.00 36.47 A 1800 CA **ASP A 300** 93.954 36.582 -9.680 **ATOM** 1.00 42.34 A -9.931 **ASP A 300** 94.782 37.845 MOTA 1801 CB 38.644 -8.666 1.00 46.20 A 1802 CG **ASP A 300** 95.014 MOTA 1.00 49.27 A 38.085 -7.719 25 OD1 ASP A 300 95.607 MOTA 1803 OD2 ASP A 300 94.599 39.826 -8.615 1.00 49.25 A 1804 ATOM -9.188 1.00 35.61 A 94.848 35.444 ATOM 1805 C **ASP A 300** -8.002 1.00 34.48 A 94.857 35.113 1806 0 **ASP A 300** MOTA 1.00 35.02 A PHE A 301 95.602 34.854 -10.111 MOTA 1807 N CA PHE A 301 96.477 33.737 -9.781 1.00 35.94 A 30 1808 MOTA 1.00 34.28 A PHE A 301 96.501 32.700 -10.909 ATOM 1809 CB 32.167 -11.301 1.00 32.40 A PHE A 301 ATOM 1810 CG 95.156 1.00 30.50 A 94.358 32.856 -12.205 MOTA 1811 CD1 PHE A 301 30.947 -10.803 1.00 31.83 A 94.708 1812 CD2 PHE A 301 ATOM 1.00 31.48 A 1813 93.131 32.333 -12.617 35 CE1 PHE A 301 **ATOM** 1.00 31.37 A PHE A 301 93.484 30.416 -11.206 MOTA 1814 CE2 1.00 31.44 A 92.695 31.109 -12.114 MOTA 1815 CZPHE A 301 1.00 38.11 A 97.916 34.134 -9.524 ATOM 1816 С PHE A 301 PHE A 301 98.458 35.010 -10.196 1.00 39.06 A MOTA 1817 0 1.00 40.47 A PRO A 302 98.559 33.498 -8.535 40 ATOM 1818 N 32.554 -7.524 1.00 41.16 A 98.053 1819 CD PRO A 302 ATOM 1.00 41.88 A PRO A 302 99.955 33.843 -8.277 ATOM 1820 CA ~6.963 1.00 42.01 A PRO A 302 100.248 33.131 ATOM 1821 CB 1.00 41.79 A 99.328 31.947 -7.001 MOTA 1822 CG PRO A 302 1.00 44.54 A 1823 -PRO A 302 100.721 33.265 -9.458 45 **ATOM** C · 32.305 -10.082 1.00 44.30 A 100.263 MOTA 1824 0 PRO A 302 1.00 47.35 A **GLU A 303** 101.874 33.843 -9.770 1825 MOTA N ATOM 1826 CA **GLU A 303** 102.667 33.395 -10.912 1.00 50.51 A 1.00 53.23 A **GLU A 303** 103.859 34.337 -11.105 MOTA 1827 CB 34.376 -12.520 1.00 56.85 A 104.431 50 MOTA 1828 CG **GLU A 303** 1.00 59.62 A 103.976 35.600 -13.314 **GLU A 303** MOTA 1829 CD 1.00 60.43 A OE1 GLU A 303 104.508 35.819 -14.424 1830 MOTA 1.00 60.45 A MOTA 1831 OE2 **GLU A 303** 103.088 36.341 -12.834 1.00 50.70 A 103.173 31.950 -10.829 ATOM 1832 **GLU A 303** C 1.00 52.21 A 103.692 31.423 -11.815 GLU A 303 55 ATOM 1833 0 ATOM ALA A 304 103.018 31.309 -9.672 1.00 49.61 A 1834 N 1.00 49.10 A ALA A 304 103.495 29.933 -9.488 ATOM 1835 CA 1.00 48.82 A ATOM 1836 ALA A 304 104.077 29.779 -8.082 CB 1.00 47.90 A 102.422 28.869 -9.713 ATOM 1837 C ALA A 304

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	ATOM	1838	· 0	ALA A	304	102.703	27.666 -9.719	1.00 49.41 A
	ATOM	1839	N	PHE A	305	101.192	29.322 -9.899	1.00 44.69 A
	ATOM	1840	CA	PHE A	305	100.053	28.440 -10.089	1.00 40.05 A
	ATOM	1841	CB	PHE A		98.809	29.301 -10.299	1.00 39.69 A
5	ATOM	1842	CG	PHE A		97.568	28.729 -9.697	1.00 37.21 A
-	ATOM	1843		PHE A		96.824	27.775 -10.379	1.00 35.36 A
	ATOM	1844		PHE A		97.133	29.157 -8.445	1.00 37.52 A
	ATOM	1845		PHE A		95.658	27.255 -9.825	1.00 34.59 A
		1846		PHE A		95.963	28.641 -7.880	1.00 37.01 A
10	ATOM ATOM	1847	CZ	PHE A		95.226	27.688 -8.575	1.00 35.13 A
10			C	PHE A		100.197	27.435 -11.230	1.00 37.65 A
	ATOM	1848		PHE A		100.364	27.814 -12.389	1.00 36.24 A
	ATOM	1849	0				26.150 -10.892	1.00 35.64 A
	ATOM	1850	N	PHE A		100.120	25.081 -11.884	1.00 33.01 A 1.00 32.40 A
1.5	ATOM	1851	CA	PHE A		100.219	23.749 -11.268	1.00 32.40 A 1.00 29.92 A
15	ATOM	1852	CB	PHE A		99.781		1.00 29.92 A 1.00 28.24 A
٠.	ATOM	1853	CG	PHE A		100.412		
	MOTA	1854		PHE A		101.796	23.457 -9.770	1.00 27.43 A
	MOTA	1855		PHE A		99.617		1.00 28.59 A
	MOTA	1856		PHE A		102.380	23.181 -8.526	1.00 29.55 A
20	ATOM	1857		PHE A		100.188	22.895 -7.566	1.00 29.06 A
	ATOM	1858	CZ	PHE A		101.575	22.901 -7.422	1.00 29.51 A
	ATOM	1859	C	PHE A		99.296	25.452 -13.047	1.00 32.76 A
	MOTA	1860	0	PHE A		98.087	25.625 -12.861	1.00 34.51 A
	ATOM	1861	N	PRO A		99.856	25.587 -14.262	1.00 31.43 A
25	ATOM	1862	CD	PRO A	307	101.272	25.327 -14.569	1.00 30.74 A
	MOTA	1863	CA	PRO A		99.128	25.947 -15.485	1.00 29.54 A
	ATOM	1864	CB	PRO A		100.158	25.700 -16.579	
	ATOM	1865	CG	PRO A		101.437	26.032 -15.895	1.00 30.81 A
	ATOM	1866	С	PRO A		97.826	25.193 -15.743	1.00 29.74 A
30	MOTA	1867	0	PRO A	,	96.795	25.804 -16.022	1.00 31.08 A
	ATOM	1868	N	LYS A		97.867	23.870 -15.660	1.00 28.47 A
	MOTA	1869	CA	LYS A		96.672	23.086 -15.904	1.00 27.92 A
	MOTA	1870	CB	LYS A		97.044	21.619 -16.114	
	MOTA	1871	CG	LYS A			21.405 -17.460	
35	MOTA	1872	CD	LYS A		98.310	20.029 -17.595	
	MOTA	1873	CE	LYS A		99.106	19.926 -18.888	
	MOŢA	1874	NZ	LYS A		99.897	18.663 -18.948	
	ATOM	1875	С	LYS A		95.632	23.247 -14.800	
	ATOM	1876	0	LYS A		94.433	23.170 -15.060	
40	MOTA	1877	N	аьа а		96.084	23.480 -13.574	
	MOTA	1878	CA	ALA A		95.145	23.685 -12.486	
	MOTA	1879	CB	ALA A		95.855	23.652 -11.146	
	MOTA	1880	C	ALA A	309	94.523	25.051 -12.712	
	MOTA	1881	0	аьа а		93.327	25.238 -12.493	
45	MOTA	1882	N	ARG A	310	95.335		
	MOTA	1883	CA	ARG A	310	94.830	27.354 -13.402	
	MOTA	1884	CB	ARG A	310	95.961	28.289 -13.864	
	ATOM	1885	CG	ARG A	310	95.438	29.584 -14.480	
	MOTA	1886	CD	ARG A	310	96.482	30.676 -14.634	
50	ATOM	1887	NE	ARG A	310	95.881	31.868 -15.233	
	MOTA	1888	CZ	ARG A	310	96.412	33.090 -15.198	
	ATOM	1889	NH1	ARG A	310	97.572	33.297 -14.588	
	MOTA	1890	NH2	ARG A	310	95.775	34.108 -15.767	
	ATOM	1891	C	ARG A		93.743	27.280 -14.473	
55	ATOM	1892	0	ARG A		92.678	27.880 -14.344	
	ATOM	1893	N	ASP A		94.019	26.524 -15.527	
	MOTA	1894	CA	ASP A		93.069	26.369 -16.615	
	MOTA	1895	CB	ASP A	311	93.682	25.504 -17.713	
	ATOM	1896	CG	ASP A	311	92.850	25.494 -18.972	1.00 35.68 A

	MOTA	1897		ASP A		91.894	24.691		38.27 A
	MOTA	1898	OD2	ASP A		93.145	26.302		37.07 A
	MOTA	1899	C	ASP A		91.769	25.748		27.22 A
	MOTA	1900	0	ASP A		90.678	26.205		29.64 A
5	ATOM	1901	N	LEU A		91.886	24.715		24.32 A
	ATOM	1902	CA	LEU A		90.708	24.062		23.48 A
	MOTA	1903	CB	LEU A		91.118	22.838		21.65 A
	MOTA	1904	CG	LEU A		90.067	22.228		21.40 A
	ATOM	1905		ĻΕU A		88.789		-13.694	16.90 A
10	MOTA	1906		TER Y		90.629		-12.294	 19.67 A
	MOTA	1907	С	LEU A		89.899		-13.871	 22.73 A
	ATOM	1908	0	LEU A		88.684		-14.021	22.02 A
	ATOM	1909	N	VAL A		90.574		-12.972	22.12 A
	ATOM	1910	CA	VAL A		89.897		-12.108	21.16 A
15	ATOM	1911	CB	VAL A		90.893		-11.167	23.49 A
	ATOM	1912		VAL A		90.221		-10.534	20.45 A
	MOTA	1913	CG2	VAL A		91.369		-10.080	21.63 A
	ATOM	1914	C	VAL A		89.161		-12.920	22.93 A
	MOTA	1915	0	VAL A		88.051		-12.566	21.46 A
20	ATOM	1916	N	GLU A		89.784		-14.001	23.15 A
	MOTA	1917	CA	GLU A		89.156		-14.832	25.95 A
	MOTA	1918	CB	GLU A		90.127		-15.900	28.61 A
	MOTA	1919	CG	GLU A		91.319		-15.350	32.73 A
	MOTA	1920	CD	GLU A		92.205		-16.453	35.94 A
25	MOTA	1921		GLU A		92.188		-17.554	40.67 A
	MOTA	1922		GLU A		92.923		-16.225	37.73 A
	ATOM	1923	C	GLU A		87.891		-15.505	24.64 A
	ATOM	1924	0	GLU A	•	87.030		-15.892	24.01 A
	MOTA	1925		LYS A		87.775		-15.654	23.67 A
30	MOTA	1926	CA	LYS A		86.588		-16.278	23.15 A 24.76 A
	MOTA	1927		LYS A		86.937		-17.042	24.70 A 22.90 A
	MOTA	1928	CG	LYS A		87.784		-18.299	23.63 A
	ATOM	1929	CD	LYS A		88.223		-18.929 -20.153	23.20 A
	ATOM	1930	CE	LYS A		89.079		-21.142	29.09 A
35∙	ATOM	1931	NZ	LYS A		88.332			23.08 A
	MOTA	1932	C	LYS A		85.509		-15.244 -15.596	23.63 A
	MOTA	1933	0	LYS A		84.386		-13.969	21.74 A
	MOTA	1934	N	LEU A		85.852		-12.876	21.74 A
	ATOM	1935	CA	LEU A		84.910		-12.876	20.54 A
40	MOTA	1936	CB	LEU A		85.569		-12.090	20.69 A
	ATOM	1937	CG	LEU A		85.841		-10.947	17.08 A
	MOTA	1938		LEU A		86.600		-12.336	19.15 A
	ATOM	1939		LEU A		84.514		-12.312	23.66 A
	ATOM	1940	C	LEU A		84.404			25.40 A
45		1941	0	LEU A		83.215		-12.013 -12.149	24.48 A
	ATOM	1942	N	LEU A		85.310	28.010	-11.637	25.52 A
	ATOM	1943	CA	LEU A		84.933	30.121	-10.936	24.23 A
	ATOM	1944	СВ	LEU A		86.123	30.733	-9.719	21.22 A
	MOTA	1945	'CG	LEU A		86.656		-9.015	23.73 A
50	ATOM	1946		L LEU A		87.718	30.859	-8.773	21.36 A
	MOTA	1947		LEU A		85.515	29.730	-12.815	26.00 A
	MOTA	1948	C	LEU A		84.459	30.955	-13.286	28.02 A
	MOTA	1949	0	LEU A		85.148	31.030	-13.293	27.50 A
	ATOM	1950	N	VAL A		83.272 82.643	31 284	-14.421	28.43 A
55	ATOM	1951	CA	VAL A		82.365		-15.558	28.13 A
	ATOM	1952	CB	VAL A VAL A		81.624		-16.694	29.20 A
	MOTA	1953		VAL A		83.677	29.689	-16.045	27.12 A
	ATOM	1954		VAL A		81.331		-13.896	29.21 A
	MOTA	1955	С	VAL A	310				

	ATOM	1956	0	VAL	A	318	80.5	59 31.120	-13.255	1.00	30.06	A
	MOTA	1957	N .	LEU	Α	319	81.0	33.121	-14.150	1.00	29.94	Α
	ATOM	1958	CA	LEU	A	319	79.8	58 33.758	-13.671	1.00	30.57	Α
	ATOM	1959	CB	LEU	Α	319	79.8	08 35.214	-14.133	1.00	32.89	A
5	MOTA	1960	CG	LEU	Α	319	80.9	08 36.115	-13.553	1.00	35.26	A
	ATOM	1961	CD1	LEU	Α	319	80.7	41 37.551	-14.059	1.00	34.63	Α
	MOTA	1962	CD2	LEU	Α	319	80.8	35 36.078	-12.028	1.00	34.01	A
	ATOM	1963	С	LEU	Α	319	78.5	98 33.029	-14.117	1.00	30.01	A
	ATOM	1964	0	LEU	Α	319	77.7	04 32.768	-13.316	1.00	30.48	A
10	ATOM	1965	N	ASP	Α	320	78.5	27 32.695	-15.397	1.00	30.13	A
	ATOM	1966	CA	ASP			77.3	62 31.996	-15.919	1.00	29.97	Α
	ATOM	1967	СВ	ASP	Α	320	77.3	93 31.981	-17.444	1.00	32.99	Α
	ATOM	1968	CG	ASP			76.1	16 31.435	-18.040	1.00	36.86	A
	ATOM	1969		ASP			75.4	95 30.548	-17.412	1.00	38.81	A
15	ATOM	1970		ASP			75.7	39 31.883	-19.142	1.00	38.26	Α
	ATOM	1971	C.	ASP			77.3		-15.402	1.00	28.61	Α
	ATOM	1972	0	ASP			78.2		-15.758	1.00	28.87	A
	ATOM	1973	N	ALA			76.3		-14.566	1.00	28.88	A
	ATOM	1974	CA	ALA			76.3		-13.980	1.00	28.04	Α
20	ATOM	1975	CB	ALA			75.1		-12.990	1.00	25.11	Α
20	ATOM	1976	C	ALA			76.1		-15.021	1.00	27.83	A
	ATOM	1977	ō	ALA			76.5		-14.773	1.00	27.26	Α
	ATOM	1978	N	THR			75.6		-16.190	1.00	27.45	Α
	ATOM	1979	CA	THR			75.4		-17.243		27.18	
25	MOTA	1980	CB	THR			74.2		-18.191		26.99	
23	ATOM	1981		THR			74.7		-18.940	1.00	27.15	Α
	ATOM	1982		THR			73.0		-17.399	1.00	23.11	Α
	ATOM	1983		THR			76.6		-18.077	1.00	28.31	A
	ATOM	1984	ō	THR			76.6		-19.027	1.00	28.80	Α
30 `	MOTA	1985	N	LYS			77.7		-17.727	1.00	28.30	A
50	ATOM	1986	CA	LYS				90 27.348		1.00	28.51	A
	ATOM	1987	CB	LYS			79.3		-19.172		30.27	
	MOTA	1988	CG	LYS			78.3		-20.095		35.72	
•		1989	CD	LYS			78.8		-21.170		37.65	
35	ATOM ATOM	1990	CE	LYS			77.7		-22.131		39.59	
33		1991	NZ	LYS			77.0		-22.733		40.41	
	ATOM	1992	C	LYS			80.1		-17.683			
	ATOM ATOM	1993	0			323	81.2		-18.119		29.54	
		1994	N.	ARG			79.8		-16.503		27.43	
40	ATOM ATOM	1995	CA	ARG			80.9		-15.684		25.01	
40		1996	CB	ARG			80.5		-14.205		22.81	
	ATOM		CG	ARG			80.4		-13.715		21.68	
	MOTA	1997 1998	CD	ARG			80.0		-12.277		20.65	
	ATOM	1999	NE	ARG			79.6		-11.971		21.18	
45	ATOM			ARG			78.6		-11.180		19.20	
45	ATOM	2000	CZ	ARG			77.9		-10.598		19.05	
	ATOM	2001		ARG			78.3		-11.004		19.45	
	MOTA	2002		ARG			81.1		-16.073		24.64	
	ATOM	2003	C .	ARG			80.2		-16.290		23.78	
50	ATOM	2004	0	LEU			82.4		-16.177		23.92	
50	MOTA	2005	N	LEU			82.8		-16.526		25.53	
	MOTA	2006	CA			325	84.3	_	-16.558		25.18	
	MOTA	2007	CB			325	84.5		-17.149		25.63	
	MOTA	2008	CG	LEU			84.5		-18.590		25.39	
<i></i>	MOTA	2009							-17.087		23.10	
55	MOTA	2010		LEU			86.5		-15.466		25.01	
	ATOM	2011	C			325	82.2		-14.278		23.83	
	MOTA	2012	0			325	82.4		-15.900		26.41	
	MOTA	2013	N			326	81.4		-15.900		26.13	
	MOTA	2014	CA	GTrA	A	326	80, 8	20 19.683	-14.204	1.00	20.13	,

		0015	_		_						
	ATOM	2015	С	GLY				79.338		-14.835	1.00 29.31 A
	MOTA	2016	0			326		78.697		-14.444	1.00 31.67 A
	ATOM	2017	N	CYS				78.753		-15.162	1.00 29.49 A
	ATOM	2018	CA	CYS				77.308		-15.042	1.00 31.91 A
5	ATOM	2019	CB	CYS	Α	327		76.935	22.556	-14.982	1.00 31.78 A
	ATOM	2020	SG			327		77.084	23.397	-16.552	1.00 38.33 A
	ATOM	2021	С	CYS	Α	327		76.539	20.385	-16.175	1.00 32.76 A
	MOTA	2022	0	CYS	Α	327		77.096	20.069	-17.228	1.00 32.18 A
	ATOM	2023	N	GLU	A	328		75.248	20.175	-15.952	1.00 33.60 A
10	MOTA	2024	CA	GLU	A	328		74.400	19.497	-16.921	1.00 36.82 A
	ATOM	2025	CB	GLU	Α	328		72.951	19.479	-16.408	1.00 41.60 A
	ATOM	2026	CG	GLU	Α	328		72.845	19.437	-14.863	1.00 48.96 A
	ATOM	2027	CD	GLU				72.000	18.279	-14.321	1.00 51.75 A
	ATOM	2028	OE1	GLU						-14.509	1.00 52.77 A
15	ATOM	2029	OE2	GLU				70.948		-13.696	1.00 52.29 A
	ATOM	2030	C	GLU				74.466		-18.317	1.00 35.83 A
	ATOM	2031	ō	GLU				74.618		-19.318	1.00 34.85 A
	ATOM	2032		GLU				74.370		-18.378	1.00 33.75 A
-	ATOM	2033	CA	GLU				74.399		-19.650	1.00 32.37 A
20	ATOM	2034	CB			329.		74.153		-19.439	1.00 32.37 A
20	ATOM	2035	CG	GLU				72.898		-18.640	1.00 34.70 A
	MOTA	2035	CD	GLU						-17.172	
		2036		GLU		-		73.017			1.00 41.60 A
	MOTA							74.048		-16.548	1.00 44.03 A
25	MOTA	2038	OE2					72.080		-16.636	1.00 44.74 A
25	ATOM	2039	C	GLU				75.711		-20.399	1.00 30.96 A
	ATOM	2040	0	GLU				75.757		-21.617	1.00 28.90 A
	ATOM	2041	N	MET				76.773		-19.673	1.00 29.20 A
	ATOM	2042	CA	MET				78.075		-20.291	1.00 27.90 A
	MOTA	2043	CB	MET				79.190		-19.455	1.00 30.57 A
30	MOTA	2044	CG	MET				79.189		-19.446	1.00 32.33 A
	ATOM	2045	SD	MET				79.488		-21.070	1.00 36.55 A
	ATOM	2046	CE	MET				81.257		-21.239	1.00 35.61 A
	MOTA	2047	C	MET				78.319		-20.443	1.00 27.32 A
	MOTA	2048	0	MET				79.452	19.436	-20.606	1.00 25.82 A
35	MOTA	2049	N	GLU	Α	331		77.232	19.122	-20.365	1.00 25.18 A
	MOTA	2050	CA	GLU	Α	331		77.246	17.677	-20.526	1.00 24.56 A
	MOTA	2051	CB	GLU	А	331		77.922	17.295	-21.848	1.00 23.55 A
	MOTA	2052	CG	GLU	Α	331		77.395	18.099	-23.030	1.00 25.42 A
	ATOM	2053	CD	GLU	Α	331		75.867	18.176	-23.082	1.00 28.50 A
40	ATOM	2054	OE1	GLU	Α	331	`	75.338	19.094	-23.750	1.00 31.00 A
	MOTA	2055	OE2	GLU	A	331		75.190	17.323	-22.467	1.00 30.18 A
	MOTA	2056	C	GLU	А	331		77.804	16.834	-19.396	1.00 24.55 A
	MOTA	2057	ο ΄	GLU	A	331		78.327	15.745	-19.629	1.00 25.02 A
	ATOM	2058	N	GLY	Α	332		77.692	17.339	-18.172	1.00 22.83 A
45	ATOM	2059	CA	GLY	Α	332		78.098	16.564	-17.017	1.00 20.57 A
	MOTA	2060	С	GLY				79.541		-16.606	1.00 20.81 A
	MOTA	2061	0	GLY	Α	332		80.430			1.00 19.36 A
	ATOM	2062	N	TYR	Α	333		79.753	15.374	-15.801	1.00 20.19 A
-	ATOM	2063	CA	TYR	A	333		81.053		-15.243	1.00 20.12 A
50	ATOM	2064	СВ	TYR				80.860		-14.052	1.00 20.05 A
	ATOM	2065	CG	TYR	Α	333		80.483		-12.828	1.00 21.40 A
	ATOM	2066		TYR				81.464		-11.956	1.00 22.85 A
	MOTA	2067		TYR				81.141		-10.878	1.00 22.91 A
	MOTA	2068		TYR				79.160		-12.590	1.00 21.24 A
55	ATOM	2069		TYR				78.827		-11.518	1.00 22.71 A
	ATOM	2070	CZ	TYR'				79.827		-10.670	1.00 21.44 A
	ATOM	2071 [.]	OH	TYR				79.522		-9.621	1.00 24.72 A
	ATOM	2072	C	TYR				82.076		-16.192	1.00 24.72 A
	ATOM	2073	Ö	TYR				83.277		-15.910	1.00 18.82 A
		· -	_								

	ATOM	2074	N	GLY	Α	334		81.610	13.942	-17.313	1.00	20.41	Α
	ATOM	2075	CA	GLY	Α	334		82.534	13.378	-18.280	1.00	20.48	Α
	ATOM	2076	С	GLY	Α	334		83.611.	14.367	-18.693	1.00	20.12	A
	MOTA	2077	0	GLY	Α	334	•	84.808	14.105	-18.539	1.00	21.13	Α
5	MOTA	2078	N	PRO	A	335		83.216		-19.230		19.75	
	ATOM	2079	CD	PRO	Α	335		81.872	15.899	-19.699	1.00	19.25	A
	ATOM	2080	CA	PRO	Α	335		84.218	16.512	-19.644		19.66	
	ATOM	2081	CB	PRO	A	335		83.366	17.644	-20.212		17.92	
	ATOM	2082	CG	PRO	Α	335		82.184	16.901	-20.784		19.24	
10	ATOM	2083	C	PRO				85.115		-18.495		19.62	
	MOTA	2084	0	PRO	Α	335		86.315	-	-18.679		21.87	
	MOTA	2085	N	LEU	A	336		84.538	17.131	-17.307		19.91	
	MOTA	2086	CA	LEU	A	336		85.312		-16.147		19.06	
	MOTA	2087	CB	LEU	Α	336		84.406		-14.914		18.05	
15	MOTA	2088	CG	LEU	Α	336		85.073		-13.571		18.25	
	MOTA	2089	CD1	TEA			•	86.049		-13.746		15.57	
	ATOM	2090	CD2	LEU				84.009		-12.538		15.31	
	MOTA	2091	· C	LEU				86.424		-15.832		17.85	
	MOTA	2092	0	LEU				87.582		-15.690		17.14	
20	MOTA	2093	N	LYS				86.075		-15.732		17.96	
	MOTA	2094	CA	LYS				87.061		-15.438		19.15	
	MOTA	2095	CB	LYS				86.352		-15.134		21.53	
	MOTA	2096	CG	LYS				85.571		-13.821		25.58	
	MOTA	2097	CD	LYS				84.484		-13.715		26.69	
25	MOTA	2098	CE	LYS				85.063	_	-13.571		29.78	
	MOTA	2099	NZ	LYS				83.979		-13.368		30.74	
	MOTA	2100	C	LYS				88.065		-16.576		21.13	
	ATOM	2101	0	LYS				89.170		-16.362		21.55	
20	MOTA	2102	N	ALA				87.697 88.600		-17.780 -18.922		22.23	
30	ATOM	2103	CA	ALA				87.802		-20.221		21.66	
	ATOM	2104	CB	ALA				89.604		-18.988		23.04	
	MOTA	2105	С. О	ALA ALA				90.518		-19.800		22.63	
	MOTA	2106 2107	N	HIS				89.447		-18.131		23.26	
35	ATOM ATOM	2107	CA	HIS				90.362		-18.148		23.33	
33	ATOM	2109	CB	HIS			-	90.017		-17.027		22.99	
	ATOM	2110	CG			339		90.696		-17.156		23.43	
	MOTA	2111		HIS				90.279		-17.710	1.00	24.32	A
	ATOM	2112		HIS				91.993		-16.741	1.00	22.64	A
40	ATOM	2113		HIS				92.346		-17.036	1.00	24.03	A
-10	MOTA	2114		HIS				91.324		-17.626	1.00	23.65	A
	ATOM	2115	C	-		339		91.833	17.302	-18.046	1.00	24.36	À
	ATOM	2116	Ö			339		92.186	16.376	-17.317	1.00	24.27	A
	ATOM	2117	N	PRO	Α	340		92.713	17.999	-18.788	1.00	25.89	Α
45	MOTA	2118	CD	PRO	Α	340		92.394	19.050	-19.777	1.00	26.27	A
	ATOM	2119	CA			340		94.151	17.714	-18.785		26.69	
	ATOM	2120	CB	PRO	Α	340		94.727	18.861	-19.613	.1.00	26.46	A
	ATOM	2121	CG	PRO	Α	340		93.654	19.090	-20.636		25.56	
	MOTA	2122	C	PRO	Α	340		94.772	17.629	-17.396	1.00	27.13	Α
50	ATOM	2123	0	PRO	A	340		95.686		-17.167		28.89	
	ATOM	2124	N			341		94.281		-16.466		26.76	
	MOTA	2125	CA	PHE	Α	341		94.815	_	-15.110		25.83	
	MOTA	2126	CB			341		94.100		-14.239		24.58	
	MOTA	2127	CG			341		94.628		-12.835		23.75	
55	· MOTA			PHE				95.890		-12.578		24.62	
	MOTA	2129		PHE				93.867		-11.765		24.82	
	MOTA	2130		PHE				96.386		-11.273		23.48	
	MOTA	2131		PHE				94.352		-10.454		23.61	
	MOTA	2132	CZ	PHE	Α	341		95.614	19.673	-10.209	T.00	23.80	A

	MOTA	2133	С	PHE A	341		94.684	17.039 -	14.458	1.00 2	5.53 I	Ą
	MOTA	2134	0	PHE A	341		95.453	16.698 -	13.572	1.00 2	5.60 A	4
	ATOM	2135		PHE A			93.718	16.248 -	14.905	1.00 2	6.56 7	Ą
•	ATOM	2136	CA	PHE A			93.486	14.928 -	-14.327	1.00 2	8.32	A
5	MOTA	2137	CB	PHE A			91.992	14.724 -	-14.095		5.63 2	
ر				PHE A			91.374	15.731 -		1.00 2	24.19 2	A.
	MOTA	2138	CG	PHE A			91.830	15.868			4.72	
	ATOM	2139					90.285	16.492			1.46	
	MOTA	2140		PHE A				16.744			22.95	
	MOTA	2141		PHE A			91.200				19.82	
10	MOTA	2142		PHE F			89.649	17.368			20.87	
	MOTA	2143	CZ	PHE A			90.105	17.491				
	MOTA	2144	C	PHE A	4 342		94.009	13.811			31.08	
	MOTA	2145	0	PHE A	342		93.655	12.643			32.72	
	ATOM	2146	N	GLU A	343	•	94.863	14.183			33.50	
15	MOTA	2147	CA	GLU A	4 343		95.446	13.250	-17.114		36.10	
	ATOM	2148	CB	GLU A	343		96.738	13.853	-17.676		38.76	
	ATOM	2149	CG	GLU A	A 343	,	96.842	13.883	-19.194	1.00 4	44.39	A
	ATOM	2150	CD		A 343		96.911	15.307	-19.750	1.00 4	48.43	A
	ATOM	2151		GLU 2			97.665	16.143	-19.190	1.00 4	47.87	A
.20	ATOM	2152	OE2		A 343		96.217	15.587	-20.755	1.00 4	49.34	Α
. 20		2152	C		A 343		95.747	11.855	-16.552	1.00	35.54	A
	ATOM		0		A 343		95.210		-17.019	1.00	33.70	Α
	ATOM	2154			A 344		96.604		-15.539	1.00	34.66	A
	ATOM	2155	N.				97.024		-14.950		33.91	
	MOTA	2156	CA		A 344		98.421		-14.360		33.13	
25	MOTA	2157	CB		A 344				-13.242		30.32	
	ATOM	2158	OG		A 344		98.387		-13.886		33.50	
	MOTA	2159	С		A 344		96.116		-13.234		32.98	
	MOTA	2160	0		A 344		96.510				31.80	
	ATOM	2161	И		A 345		94.908		-13.713		31.70	
30	ATOM	2162	CA	VAL .	A 345		94.021		-12.689		31.20	
	MOTA	2163	CB	VAL	A 345		93.039		-12.152		29.96	
	ATOM	2164	CG1	VAL	A 345		92.153		-11.079			
	ATOM	2165	CG2	VAL	A 345		93.799		-11.601		27.23	
	ATOM	2166	G	VAL	A 345		93.175		-13.133		32.88	
35	ATOM	2167	φ	VAL	A 345		92.597		-14.223		32.39	
	ATOM	2168	Ŋ	THR	A 346		93.109		-12.279		31.88	
	ATOM	2169	CA	THR	A 346		92.285		-12.539		32.94	
	ATOM	2170	CB	THR	A 346		93.007	5.209	-12.149		35.61	
	ATOM	2171			A 346		94.137	5.012	-13.013		37.85	
40	ATOM	2172	CG2		A 346		92.060	4.022	-12.267	1.00	32.32	A
40	MOTA	2173	C		A 346		91.051	6.700	-11.658		33.08	
		2174	ō		A 346		91.083	6.460	-10.448	1.00	34.21	Α
	ATOM	2175	И.		A 347		89.964		-12.274	1.00	31.78	A
	ATOM	2176	CA		A 347		88.741		-11.549	1.00	31.53	Α
	MOTA				A 347		97 769	8.171	-12.463		28.28	
45	ATOM	2177	CB				88.303	9 476	-12.937		23.66	
	ATOM	2178	CG		A 347		88.263		-12.231		23.03	
	MOTA	2179			A 347				-13.031		20.77	
	MOTA	2180			A 347		88.927		-10.999		20.57	
	MOTA	2181			A 347		87.731				21.92	
50	MOTA	2182			A 347		88.969		-14.102		22.23	
	MOTA	2183	NE		A 347		89.348		-14.168		21.04	
	MOTA	2184			A 347		89.074		-12.640		20.11	
	MOTA	2185			A 347		87.876		-10.611			
	ATOM	2186	CH:	2 TRP	A 347		88.544		-11.430		20.44	
55	ATOM	2187	C	TRP	A 347		88.014		-10.899		34.19	
	ATOM	2188		TRP	A 347		87.382		-9.854		34.97	
	ATOM	2189		GLU	A 348		88.108		-11.502		35.77	
	ATOM	2190			A 348		87.405		-11.000		36.41	
	ATOM	2191			A 348		87.600	2.740	-11.977	1.00	36.95	, A

2.626 -12.588 0.00 36.86 A 88.990 ATOM 2192 CG **GLU A 348** 0.00 36.91 A 89.173 3.510 -13.812 CD **GLU A 348** ATOM 2193 4.750 -13.677 0.00 36.92 A 2194 OE1 GLU A 348 89.119 ATOM 0.00 36.92 A 2.960 -14.916 ATOM 2195 · OE2 **GLU A 348** 89.370 -9.563 1.00 36.38 A 87.668 3.435 2196 C **GLU A 348** MOTA 2.866 -8.935 1.00 38.29 A 86.773 **GLU A 348** MOTA 2197 0 -9.019 1.00 34.41 A **ASN A 349** 88.857 3.669 2198 N MOTA -7.668 1.00 33.02 A 3.182 CA **ASN A 349** 89.134 ATOM 2199 -7.765 1.00 34.07 A 89.848 1.844 2200 CB **ASN A 349** ATOM -8.381 1.00 35.48 A CG **ASN A 349** 91.220 1.978 10 MOTA 2201 2.742 -9.324 1.00 35.13 A 91.409 ATOM 2202 OD1 ASN A 349 ND2 ASN A 349 -7.852 1.00 38.04 A 92.188 1.235 MOTA 2203 1.00 30.73 A C **ASN A 349** 89.970 4.116 -6.804 MOTA 2204 -6.106 1.00 30.66 A **ASN A 349** 90.878 3.672 ATOM 2205 0 5.403 -6.850 1.00 28.42 A 89.662 2206 N **LEU A 350** 15 ATOM -6.072 1.00 27.13 A **LEU A 350** 90.390 6.397 MOTA 2207 CA 89.655 7.737 -6.128 1.00 25.19 A LEU A 350 ATOM 2208 CB -7.418 1.00 25.97 A 89.803 8.543 2209 CG LEU A 350 ATOM 1.00 26.30 A 9.732 -7.428 2210 CD1 LEU A 350 88.841 MOTA 9.014 -7.521 1.00 27.40 A 91.242 20 ATOM 2211 CD2 LEU A 350 ,-4.614 1.00 26.30 A С LEU A 350 90.581 5.999 ATOM 2212. 0 **LEU A 350** 91.645 6.201 -4.036 1.00 26.73 A 2213 MOTA 1.00 27.16 A -4.024 89.547 5.424 ATOM 2214 N HIS A 351 -2.622 1.00 28.60 A 5.044 HIS A 351 89.593 MOTA 2215 CA 1.00 29.94 A 4.748 -2.124 HIS A 351 88.184 25 MOTA 2216 CB 88.111 4.503 -0.653 1.00 30.99 A HIS A 351 MOTA 2217 CG 0.399 1.00 31.86 A 88.324 5.329 2218 CD2 HIS A 351 MOTA -0.118 1.00 29.43 A ND1 HIS A 351 87.790 3.275 MOTA 2219 87.804 1.00 31.81 A 3.356 1.202 CEL HIS A 351 MOTA 2220 NE2 HIS A 351 88.125 4.592 1.541 1.00 32.90 A 30 2221 ATOM 1.00 28.99 A 90.509 3.873 -2.298 MOTA 2222 C HIS A 351 1.00 28.53 A 90.875 3.677 -1.141 MOTA 2223 0 HIS A 351 90.865 3.088 -3.307 1.00 30.57 A **GLN A 352** MOTA 2224 N -3.095 1.00 33.42 A 91.764 1.959 **GLN A 352** MOTA 2225 CA 1.00 35.01 A 91.563 0.880 -4.162 GLN A 352 35 MOTA 2226 CB 1.00 37.07 A **GLN A 352** 90.696 -0.289 -3.737 2227 CG ATOM 1.00 39.83 A 0.123 -3.474 MOTA 2228 CD **GLN A 352** 89.275 88.676 1.00 41.90 A 0.856 -4.267 ATOM 2229 OE1 GLN A 352 NE2 GLN A 352 88.712 -0.351 -2.365 1.00 39.86 A 2230 MOTA 1.00 33.85 A -3.173 GLN A 352 93.197 2.457 40 ATOM 2231 C -2.734 1.00 35.32 A 1.782 0 GLN A 352 94.126 MOTA 2232 GLN A 353 ' 93.368 3.647 -3.7341.00 32.53 A ATOM 2233 N GLN A 353 -3.886 1.00 32.78 A 94.693 4.216 MOTA 2234 CA 1.00 32.07 A 94.666 5.298 -4.965 **GLN A 353** 2235 CB ATOM 1.00 31.94 A **GLN A 353** 94.373 4.739 -6.345 MOTA 2236 CG 45 -7.382 1.00 32.50 A 94.206 5.819 ATOM 2237 CD **GLN A 353** 1.00 35.33 A 95.008 6.749 -7.452 OE1 GLN A 353 ATOM 2238 NE2 GLN A 353 93.167 5.701 -8.204 1.00 31.02 A 2239 MOTA 1.00 33.27 A 95.246 4.779 -2.588 MOTA 2240 C **GLN A 353** 1.00 32.38 A -1.717 GLN A 353 94.494 5.209 50 ATOM 2241 0 1.00 33.29 A -2.462 96.570 4.746 MOTA 2242 N THR A 354 THR A 354 97.239 5.267 -1.280 1.00 34.35 A MOTA 2243 CA 1.00 35.88 A THR A 354 98.615 4.601 ~1.069 MOTA 2244 CB 1.00 36.70 A -0.690 OG1 THR A 354 98.430 3.232 ATOM 2245 99.403 1.00 36.08 A 0.027 5.325 55 ATOM 2246 CG2 THR A 354 1.00 33.06 A 97.440 6.760 -1.478 C THR A 354 2247 ATOM 1.00 31.33 A 98.120 7.181 -2.403 2248 0 THR A 354 ATOM 1.00 33.40 A PRO A 355 96.844 7.581 -0.604 MOTA 2249 N 1.00 31.90 A 96.000 7.220 0.544 MOTA 2250 CD PRO A 355

	ATOM	2251	CA	PRO 2	A.	355		96.974	9.035	-0.710	1.00	34.90	A
	ATOM	2252	CB	PRO 2	A	355		96.156	9.543	0.475	1.00	33.68	Α
	ATOM	2253	CG	PRO 2	Α	355		95.160	8.452	0.698	1.00	33.37	Α
	ATOM	2254	С	PRO 2	A	355		98.428	9.475	-0.623	1.00	36.27	Α
5	MOTA	2255	0	PRO .	A	355		99.196	8.960	0.191	1.00	35.70	A
-	ATOM	2256	N	PRO .				98.824	10.433	-1.464	1.00	37.66	A
	ATOM	2257	CD	PRO .	A	356		98.010	11.198	-2.423	1.00	38.22	A
	ATOM	2258	CA	PRO				100.205	10.916	-1.441	1.00	39.93	Α
	ATOM	2259	CB	PRO .				100.227	11.944	-2.570	1.00	38.83	Α
10	ATOM	2260	CG	PRO				98.818	12.466	-2.580	1.00	38.26	Α
	ATOM	2261	C	PRO				100.532	11.534	-0.085	1.00	41.87	A
	ATOM	2262	O	PRO	Α	356		99.696	12.209	0.506	1.00	40.91	Α
	ATOM	2263	N	ALA				101.741	11.286	0.409	1.00	46.23	Α
	ATOM	2264	CA	ALA	A	357		102.160	11.837	1.691	1.00	51.16	A
15	ATOM	2265	CB	ALA	A	357		103.587	11.410	2.001	1.00	49.78	Α
	ATOM	2266	С	ALA				102.077	13.354	1.589	1.00	54.64	A
	ATOM	2267	0	ALA				102.591	13.942	0.637	1.00	55.14	Α
	ATOM	2268	N	LEU				101.419	13.985	2.559	1.00	58.59	A
	ATOM	2269	CA	LEU	A	358		101.276	15.437	2.552		62.92	
20	ATOM	2270	CB	LEU	А	358		100.107	15.866	3.441	1.00	62.51	Α
	ATOM	2271	CG	LEU	Α	358		98.732	15.752	2.783	1.00	63.05	Α
	MOTA	2272	CD1	LEU	Α	358		97.657	16.251	3.737		63.34	
	MOTA	2273	CD2	LEU	Α	358		98.721	16.570	1.494	1.00	62.56	A
	ATOM	2274	C	LEU	Α	358		102.536	16.173	2.984	1.00	65.81	A
25	ATOM	2275	0	LEU	Α	358		102.675	16.559	4.148		66.45	
	ATOM	2276	N	THR	Α	359		103.441	16.368	2.025		69.31	
	ATOM	2277	CA	THR	Α	359		104.715	17.057	2.236		72.25	
	ATOM	2278	CB	THR	А	359		104.519	18.594	2.271		73.17	
	ATOM	2279	OG1	THR	Α	359		103.564	18.937	3.284		75.38	
30	ATOM	2280	CG2	THR	Α	359		104.030	19.101	0.916		72.93	
	ATOM	2281	G.	THR	Α	359		105.468	16.627	3.497		73.76	
	ATOM	2282	0	THR				105.011	15.683	4.180		74.61	
	MOTA	2283	OXT	THR	A	359		106.523	17.237	3.780		75.50	
	MOTA	2284	OH2	TIP	s	1	•	82.965	32.402	-3.946		13.32	
35	ATOM .	2285		TIP		2		91.556		-17.557		22.11	
	MOTA	2286		TIP		3		87.391	33.155	-1.722		22.84	
	MOTA	2287	OH2	TIP	s	4		69.033	3.499	13.879		22.91	
	MOTA	2288		TIP		5		81.088		-18.406		24.13	
	ATOM	2289		TIP		6		75.641	16.130			26.44	
40	MOTA	2290		TIP		7		74.760	20.961			27.74 22.53	
	MOTA	2291		TIP		8		75.152	6.784	5.545		35.96	
	ATOM	2292	OH2		S	. 9		77.282		-17.666		25.44	
	MOTA	2293	OH2		S	10		81.785	8.968	-8.072		22.05	
	MOTA	2294		TIP		11		78.609	24.424	-2.074		37.17	
45	MOTA	2295		TIP		12		94.883		-9.981		35.95	
	MOTA	2296		TIP		13		73.164	38.970	-1.072		39.27	
	MOTA	2297		TIP		14		78.806	27.556	-3.116		23.40	
	MOTA	2298		TIP		15		89.050	8.041	10.604		26.94	
	MOTA	2299		TIP		16		73.265	40.376	-3.301		30.61	
50	MOTA	2300		TIP		18		84.081	33.371	4.243		26.61	
	MOTA	2301		TIP		19		78.571	-0.530	16.531		28.94	
	ATOM	2302		TIP		21	•	70.088	3.703	17.559 -18.791		26.94	
	MOTA	2303		TIP		22		79.212		-16.751		30.26	
	ATOM	2304		TIP				91.672 104.173	17.689	-7.204		31.65	
55	MOTA	2305		TIP				87.578		-20.604		25.98	
	ATOM	2306		TIP TIP				82.272		-16.021		27.40	
	ATOM	2307						100.496	13.074	-9.812		37.92	
	MOTA	2308		TIP				65.147	10.515	28.440		40.03	
	MOTA	2309	UHZ		ာ	. ⊃∪		JJ.111					

	ATOM	2310	ОН2	TIP	s	31	90.721	38.800	-4.631	1.00 42.09 S
	ATOM	2311	OH2	TIP	S	32	83.367	23.841	15.654	1.00 36.15 S
	ATOM	2312	OH2	TIP	s	33	87.754	11.897	23.760	1.00 26.76 S
	ATOM	2313	OH2	TIP	S	34	77.755	13.485	-15.395	1.00 31.85 S
5	ATOM	2314	OH2	TIP	S	35	79.767	43.115	5.371	1.00 35.26 S
	ATOM	2315	OH2	TIP	S	37	80.173	32.998	6.198	1.00 40.03 S
•	ATOM	2316	OH2	TIP	S	40	85.958	19.110	24.502	1.00 24.42 S
	ATOM	2317	OH2	TIP	s	42	77.719	-0.391	23.732	1.00 39.71 S
	ATOM	2318	OH2	TIP	S	44	92.563	36.428	-5.574	1.00 35.43 S
10	ATOM	2319	OH2	TIP	s	45	90.942	34.092	3.570	1.00 43.64 S
	ATOM	2320	ОН2	TIP	s	46	74.357	32.157	-13.849	1.00 33.31 S
	ATOM	2321	OH2	TIP	S	47	90.220	14.449	16.172	1.00 34.34 S
	ATOM	2322	OH2	TIP	s	48	77.876		-13.863	1.00 23.53 S
	MOTA	2323	OH2	TIP	s	50	76.289	12.589		1.00 37.74 \$
15	ATOM	2324	OH2	TIP	s	51	76.619	2.787	-2.969	1.00 35.95 S
	ATOM	2325	OH2	TIP	s	52	65.118	19.629	24.370	1.00 34.85 S
	ATOM	2326	OH2	TIP	s	53	99.690		-13.046	1.00 48.21 S
	ATOM	2327	OH2	TIP		54	88.376	36.865	3.454	1.00 38.54 S
	ATOM	2328		TIP			91.236	10.819	18.279	1.00 40.76 S
20	ATOM	2329	OH2	TIP			100.017		-14.622	1.00 41.65 S
	ATOM	2330		TIP		63	87.188	25.521	11.438	1.00 41.53 S
	ATOM	2331	OH2		s	65	90.264	19.625	12.286	1.00 24.22 S
	ATOM	2332	OH2	TIP		66	83.805		-18.365	1.00 37.50 S
	ATOM	2333	OH2	TIP		68	78.394	7.378	2.855	1.00 23.47 S
25	ATOM	2334	OH2			74	85.541		-18.436	1.00 37.35 S
	ATOM	2335		TIP		76	98.981	8.707	2.808	1.00 47.34 S
	ATOM	2336				78	87.802	19.118	22.522	
	ATOM	2337		TIP		80	92.438	3.105	2.517	1.00 37.27 S
	ATOM	2338		TIP		81	75.580	-0.821	22.186	1.00 37.27 S
30	ATOM	2339	OH2	TIP	s	82	60.506	24.278	21.938	1.00 30.11 S
	ATOM	2340	OH2			83	92.298		-21.183	1.00 42.32 S
	ATOM	2341		TIP		84	74.351	4.211	-3.464	1.00 32.53 S
•	ATOM	2342		TIP	s	85	76.502		-21.839	1.00 41.89 S
	ATOM	2343		TIP		86	97.965	13.142	9.216	1.00 41.76 S
35	ATOM	2344		TIP		87	78.657	4.418		1.00 41.70 B
,	ATOM	2345			s	88	93.633	28.572	3.429	1.00 33.03 S
	ATOM	2346	OH2			89	104.691	20.306	-7.235	1.00 34.30 S
	ATOM	2347		TIP		91	98.360		-15.558	1.00 37.92 S
	ATOM	2348		TIP	s	92	88.175		-14.088	1.00 37.32 B
40	ATOM	2349		TIP	-	93	96.974		-17.613	1.00 30.31 S
	ATOM	2350		TIP		94	85.585	22.346	15.199	1.00 34.47 5
	ATOM	2351	OH2	TIP	s	100	80.948	-0.010	7.892	1.00 41.12 S
	ATOM	2352		TIP		101	76.653	29.202	-3.527	1.00 12.04 S
	ATOM	2353		TIP			74.980	8.979	-7.975	1.00 22.10 5
45	ATOM	2354								
7,5	ATOM	2355		TIP			88.843 76.862	28.393 8.067	3.994 28.490	1.00 30.94 S 1.00 20.20 S
	ATOM	2356		TIP			66.435	30.702	8.817	1.00 20.20 S 1.00 35.87 S
	ATOM	2357		TIP				7.757	8.860	1.00 35.87 S
	ATOM	2358		TIP			67.384 66.852	4.666	22.301	1.00 39.38 S
50	ATOM	2359		TIP			72.391	2.229		1.00 32.73 S
50	ATOM	2360		TIP			80.209	7.061	-7.886	1.00 31.07 S
	ATOM	2361		TIP			74.466		-12.357	1.00 35.49 S
	ATOM	2362		TIP			79.225	28.627	0.179	1.00 45.36 S
	ATOM	2362		TIP			59.090	28.627	22.498	1.00 30.88 S
55	ATOM	2364		TIP			73.715		-13.973	1.00 35.94 S 1.00 44.35 S
J.J	ATOM	2365		TIP			105.619		-13.973	1.00 44.33 \$
	ATOM	2366		TIP					-16.090	1.00 43.80 S
	ATOM	2367		TIP			86.658 70.750		-10.875	1.00 39.40 S
	ATOM	2368		TIP				12.663	6.090	1.00 43.74 S
	1-1	2200	0.112	112	Ç	T 2 0	77.820	14.003	0.000	7.00 71.10 0

	MOTA	2369	OH2	TIP	s	142		90.942	35.947	-13.582	1.00	48.16 S	
	ATOM	2370	OH2	TIP	S	146		67.351	6.830	24.075	1.00	36.66 S	
	ATOM	2371		TIP				98.067	12.182	-7.216	1.00	38.66 S	
	ATOM	2372		TIP				75.211		-20.582	1.00	45.56 S	
5	ATOM	2373		TIP				72.261	20.575	12.175		51.45 S	
3	ATOM	2374		TIP				77.289	42.685	7.086		42.23 S	
		2374	OH2					65.330	6.552	20.003		42.22 S	
	MOTA			TIP			•	88.027		-20.665		35.09 S	
	ATOM	2376						99.488		-16.497		44.21 S	
10	MOTA	2377		TIP								50.19 S	
10	MOTA	2378	OH2	TIP				93.851		-20.448		39.52 S	
	MOTA	2379						83.811	26.388	9.460			
	MOTA	2380		TIP				91.704	42.080	2.405		40.67 S	
	ATOM	2381		GLC		1		82.624	0.887			47.94 G	
	MOTA	2382	C11	GLC	G	1		82.240	2.160	13.000		48.49 G	
15	ATOM	2383		GLC		1.		83.237	3.235	12.553		46.87 G	
	MOTA	2384	014	GLC	G	1		84.544	2.903	13.022		46.62 G	
	ATOM	2385	C15	GLC	G	1		82.817	4.591	13.117		45.80 G	
	ATOM	2386	016	GLC	G	1		83.746	5.589	12.703	1.00	43.50 G	
	ATOM	2387	012	GLC	G	5		86.722	-2.593	0.107	1.00	39.62 G	
20	ATOM	2388	C11	GLC	G	5		86.245	-1.364	-0.429	1.00	44.37 G	
	ATOM	2389	C13	GLC	G	5	-	86.764	-0.193	0.394	1.00	44.36 G	
	ATOM	2390		GLC		5		86.355	-0.326	1.761	1.00	47.64 G	
	ATOM	2391		GLC		5		86.231	1.132	-0.195	1.00	45.11 G	
	ATOM	2392		GLC		5		86.666	1.310	-1.557	1.00	42.61 G	
25	ATOM	2393		GLC		8		87.512	4.414			38.37 G	
23	ATOM	2394		GLC		8		86.362	5.220			34.16 G	
	ATOM	2395		GLC		8		85.750	5.654			35.54 G	
				GLC		8	•	86.717	6.392	-7.111		37.03 G	
	ATOM	2396		GLC		8		84.521		-6.082		35.46 G	
20	ATOM	2397				8			6.931			33.79 G	
30	ATOM	2398		GLC.				83.948				23.98 L	
	ATOM	2399		STO		1		82.178	19.404	•			
	ATOM	2400	•	STO		1		83.091	19.645			24.40 L	
	MOTA	2401		STO		1		82.557	20.621			19.84 L	
•	ATOM	2402		STO		1		83.748	21.455			20.35 L	
35	MOTA	2403		STO		1		84.251	22.242			22.56 L	
	MOTA	2404		sto		1		83.716	23.544			20.91 L	
	MOTA	2405		STO		1		84.847	20.523			19.37 L	
	MOTA	2406		STO		1		84.278	19.595			18.70 L	
	MOTA	2407	029	STO	L	1		82.889	19.845			20.08 L	
40	MOŢA	2408	C24	STO	L	1		81.939	19.930	12.872		21.85 L	
	ATOM	2409	C35	STO	L	1		80.791	20.824	13.403		20.12 L	
	MOTA	2410	N6	STO	L	1		81.456	18.689	12.528		19 _. 30 L	
	ATOM	2411	. C5	STO	L	1		80.172	18.450	12.023	1.00	16.04 L	
	MOTA	2412	C4	STO	L	1		79.039	19.219	11.690	1.00	14.17 L	
45	MOTA	2413	C3	STO	L	1		77.901	18.569	11.148	1.00	14.32 L	ı
	ATOM	2414	C2	STO		1		77.899	17.158	10.946	1.00	14.05 L	
	ATOM	2415	C1	STO		1		79.035	16.386	11.282	1.00	13.54 L	
		2416	C23			1		80.154	17.053		1.00	16.42 L	,
	ATOM	2417	C22			. 1		81.361	16.522		1.00	17.74 L	
50	ATOM	2418	C7	STO		1		82.162	17.525			18.84 L	
50	ATOM	2419	C8	STO		1		83.501	17.279			18.69 L	
	ATOM	2419	N9	STO				84.462	18.150			19.59 L	
				STO				85.663	17.477			19.11 L	
	ATOM	2421		STO		1		86.968	17.838			16.81 L	
56	ATOM	2422										20.66 L	
55	ATOM	2423		STO		1		87.961	16.831			20.30 L	
	ATOM	2424		STO				87.645	15.476			19.66 L	
	ATOM	2425		STO				86.329	15.117			19.00 L	
	MOTA	2426		STO		1		85.364	16.127			19.21 L	
	MOTA	2427	C16	STO	L	1		84.049	16.022	12.899	1.00	12.21	J

							•				
	MOTA	2428	C17	STO	L	1		83.217	14.936	12.440	1.00 18.26 L
	ATOM	2429	C21	STO	L	1		81.934	15.217	12.098	1.00 17.21 L
	MOTA	2430	C20	STO	L	1		81.325	14.098	11.689	1.00 17.68 L
	MOTA	2431	N19	STO	L	1		82.281	13.080	11.786	1.00 13.64 L
5	ATOM	2432	C18	STO	L	1		83.457	13.603	12.261	1.00 16.89 L
	MOTA	2433	030	STO	L	1		84.493	12.981	12.504	1.00 15.41 L
	ATOM	2434	S	SO4	I	1		64.914	7.877	16.247	1.00 82.11 I
	MOTA	2435	01	SO4	I	1		63.624	8.415	15.778	1.00 82.68 I
	ATOM	2436	02	SO4	I	1		65.841	8.992	16.520	1.00 82.73 I
10	ATOM	2437	О3	504	I	1		65.479	7.010	15.198	1.00 83.33 I
	ATOM	2438	04	SO4	I	1		64.709			1.00 82.04 I
	ATOM	2439	S	SO4	I	2		68.379	-7.029	19.810	
	ATOM	2440	01	S04	I	2		66.992	-6.526		
	ATOM	2441	02	SO4		2		68.850	-7.226		
15	ATOM	2442	О3	SO4	I	2		68.426	-8.312	20.538	1.00112.24 I
	ATOM	2443	04	SO4	I	2		69.249	-6.051	20.491	
	ATOM	2444	s	SO4	I	3		84.927	-1.874		
_	ATOM	2445	01	SO4	I	3		84.408	-1.334		
	ATOM	2446	02	S04	I	. 3		84.442	-1.050	•	1.00 80.43 I
20	ATOM	2447	03	SO4	I	3		84.453	-3.263		
	ATOM	2448	04	SO4	I	3		86.402	-1.845		
	ATOM	2449	S	S04	I	4		80.577	9.632		1.00 98.23 I
	ATOM	2450	01	SO4	I	4		79.725	9.060		1.00 96.88 I
	ATOM	2451	02	SO4	I	4		82.000	9.461		
25	ATOM	2452	03	SO4	I	4		80.304	8.944		
	ATOM	2453	04	S04		4		80.281	11.069		
	ATOM	2454	S	SO4		5		89.310	6.131		
	ATOM	2455	01	S04		5		89.025	6.456		
	ATOM	2456	02	S04		. 5		88.042	6.095		
30	ATOM	2457	03	SO4		5		89.970	4.810		
	ATOM		04	SO4		5		90.205	7.155		
	ATOM	2459	02	PO4		100		64.527	26.252		
	ATOM	2460	03	PO4	P	100		66.482	25.155	1.367	1.00 88.39 P
	ATOM	2461	04	PO4	P	100		66.688	26.504		·
35	ATOM	2462	01			100		66.264	27.565		
	ATOM	2463	P	P04	P	100		65.992	26.368		
	ATOM	2464	СВ	LEU		145		73.932	8.398		0.50 21.29 AC2
	MOTA	2465	CG	LEU		145		72.901	8.606		0.50 21.65 AC2
	ATOM	2466	CD1	LEU		145		71.904	9.671		0.50 21.60 AC2
40	ATOM	2467		LEU		145		72.195	7.298		0.50 19.61 AC2
	ATOM	2468	CB	ASN		214		88.968	8.625		0.50 22.34 AC2
	ATOM	2469	CG	ASN		214	-	89.705	8.084		0.50 22.01 AC2
	MOTA	2470		ASN		214		89.240	7.153		0.50 22.82 AC2
	ATOM	2471		ASN		214		90.859 `	8.660	•	0.50 22.69 AC2
45	MOTA	2472	СВ	ASP		216		93.187	5.546		0.50 25.98 AC2
	ATOM	2473	CG	ASP		216		91.789	5.828		0.50 27.09 AC2
	ATOM	2474		ASP		216		91.587	6.896		0.50 28.49 AC2
	ATOM	2475	-	ASP		216		90.896	4.982		0.50 28.20 AC2
	END									5.225	

Example 8: Co-ordinates for PDK1 fragment co-crystallised with UCN-

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.50 A
    REMARK starting r= 0.1919 free_r= 0.2582
                    r= 0.1894 free r= 0.2567
    REMARK final
    REMARK B rmsd for bonded mainchain atoms= 1.412 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.205 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.401 target= 2.0
    REMARK B rmsd for angle sidechain atoms= 3.256 target= 2.5
10
    REMARK rweight= 0.1000 (with wa= 3.1611)
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.387 b= 123.387 c= 47.115 alpha= 90 beta=
    90 gamma= 120
15
    REMARK parameter file 1 : /dd1/david/refinement/MY_CNS/prot.par
    REMARK parameter file 2 : /dd1/david/refinement/MY CNS/ucn01.par
    REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
    REMARK parameter file 4 : CNS_TOPPAR:ion.param
    REMARK parameter file 5
    /dd1/david/refinement/MY_CNS/glycerol.par
    REMARK molecular structure file: ../generate/generate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../data/cns.hkl
    REMARK ncs= none
25
    REMARK B-correction resolution: 6.0 - 2.50
    REMARK initial B-factor correction applied to fobs :
    REMARK
           B11= -4.722 B22= -4.722 B33=
                                             9.444
    REMARK
             B12= -3.572 B13=
                                 0.000 B23=
                                              0.000
    REMARK B-factor correction applied to coordinate array B:
                                                                -0.193
30
    REMARK bulk solvent: density level= 0.3837 e/A^3, B-factor=
    40.9071 A^2
    REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range: 14485 (
35
    100.0 % )
    REMARK number of unobserved reflections (no entry or |F|=0):
            0.7 % )
    101 (
    REMARK number of reflections rejected:
                                                     0 (
                                                           0.0 % )
    REMARK total number of reflections used:
                                                     14384 ( 99,3 % )
40
    REMARK number of reflections in working set:
                                                  13795 ( 95.2 % )
    REMARK number of reflections in test set:
                                                     589 ( 4.1 % )
    CRYST1 123.387 123.387
                              47.115 90.00 90.00 120.00 P 32 2 1
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE: 25-Mar-2003 17:21:21
                                            created by user: david
    REMARK VERSION:1.0
45
              1 CB ALA A 73
    ATOM
                                    67.051 -3.293 12.591
                                                            1.00 59.77 A
                     ALA A 73
    MOTA
              2
                 C
                                    67.941 -4.753
                                                    14.416
                                                            1.00 61.14 A
    MOTA
              3
                 0
                     ALA A
                            73
                                    67.184 -5.270
                                                    15.240
                                                            1.00 61.61 A
                                            -5.729
    ATOM
              4
                 N
                     ALA A
                            73
                                                    12.643
                                    66.523
                                                            1.00 58.89 A
50
                 ÇA
    ATOM
              5
                     ALA A
                            73
                                    67.564
                                            -4.697
                                                    12.943
                                                            1.00 60.69 A
              6 N
                     PRO A
                                                    14.770
                                                            1.00 61.63 A
    MOTA
                            74
                                            -4.241
                                    69.130
                 CD
                     PRO A
    MOTA
              7
                            74
                                    70.264
                                            -3.830
                                                    13.918
                                                            1.00 61.72 A
                 CA
                     PRO A 74
    MOTA
              8
                                    69.514
                                            -4.278
                                                    16.187
                                                            1.00 61.34 A
                 CB
                     PRO A
                            74
              9
                                    70.918
                                            -3.663
                                                    16.181
    ATOM
                                                            1.00 61.79 A
             10
                                    71.458
55
    ATOM ·
                 CG
                     PRO A
                            74
                                            -4.072
                                                    14.818.
                                                            1.00 61.47 A
                 C
                     PRO A
                                            -3.481
    MOTA
             11
                            74
                                    68.523
                                                    17.047
                                                             1.00 60.16 A
    ATOM
             12
                 0
                     PRO A
                            74
                                    67.625
                                            -2.817
                                                    16.519
                                                             1.00 60.77 A
```

MOTA

WO 03/104481 PCT/GB03/02509

312

18.368 1.00 58.13 A 68.680 -3.562 75 MOTA 13 N ALA A 1.00 54.74 A 67.815 -2.828 19.292 ALA A 75 CA MOTA 14 1.00 54.90 A 15 68.048 -3.309 20.731 CB ALA A 75 ATOM 1.00 51.85 A -1.349 19.177 16 С ALA A 75 68.175 ATOM 1.00 52.46 A -1.005 18.851 o ALA A 75 69.313 ATOM 17 1.00 46.96 A 67.215 -0.473 19.427 LYS A 76 MOTA 18 N 1.00 43.72 A 19.354 0.947 LYS A 76 67.507 CA ATOM 19 1.756 19.744 1.00 42.81 A 66.270 CB LYS A 76 20 MOTA 1.00 41.81 A 3.116 19.087 LYS A 76 66.177 21 CG MOTA 1.00 40.56 A 2.983 17.590 CD LYS A 76 65.926 MOTA 22 1.00 42.58 A 16.943 65.691 4.343 MOTA 23 CE LYS A 76 1.00 42.73 A 4.231 15.495 LYS A 76 65.362 NZ 24 MOTA 1.00 41.25 A 20.351 1.218 25 С LYS A 76 68.639 ATOM 1.00 41.68 A 0.741 21.488 LYS A 76 68.599 ATOM 26 0 1.00 37.68 A 69.655 1.960 19.936 27 N LYS A 77 15 MOTA 1.00 35.10 A 2.255 20.849 CA LYS A 77 70.748 MOTA 28 1.00 34.13 A 20.074 72.016 2.619 77 MOTA 29 CB LYS A 1.00 32.68 A 19.053 1.570 72.427 CG LYS A 77 30 ATOM 18.858 1.00 33.90 A 1.537 LYS A 77 73.927 31 CD MOTA 0.471 17.849 1.00 31.40 A 74.366 20 MOTA 32 CE LYS A 77 1.00 34.76 A -0.863 18.164 NZ77 73.796 LYS A MOTA 33 21.743 1.00 34.79 A LYS A 77 70.313 3.408 34 С MOTA 21.458 1.00 34.20 A 4.077 69.319 ATOM 35 0 LYS A 77 1.00 34.88 A 3.626 22.845 71.023 ARG A 78 MOTA 36 N 1.00 34.62 A 23.759 70.687 4.723 78 25 37 CA ARG A MOTA 1.00 38.43 A 24.839 ARG A 69.694 4.247 78 ATOM 38 CB 1.00 42.71 A 2.884 25.353 70.027 39 CG ARG A 78 ATOM 1.00 48.52 A 26.625 69.355 2.424 ARG A 78 ATOM 40 CD 27.412 1.00 56.10 A 1.702 70.365 MOTA 41 NE ARG A 78 1.00 57.88 A 70.428 0.355 27.518 ARG A 78 30 MOTA 42 CZ1.00 58.45 A 69.519 -0.397 26.838 NH1 ARG A 78 43 ATOM 28.369 1.00 59.23 A -0.195 NH2 ARG A 78 71.335 MOTA 44 1.00 32.26 A 5.330 24.382 71.967 ATOM 45 C ARG A 78 1.00 31.42 A 4.777 24.278 73.066 78 46 0 ARG A MOTA 1.00 30.46 A 24.997 71.844 6.509 PRO A 79 . 35 MOTA 47 N 25.232 1.00 28.96 A 70.616 7.284 PRO A 79 48 CD MOTA 1.00 30.38 A 7.172 25.609 49 CA PRO A 79 72.997 ATOM 1.00 28.86 A 26.405 72.350 8.303 50 CB PRO A 79 MOTA 1.00 27.83 A 79 71.169 8.642 25.568 PRO A CG MOTA 51 1.00 29.47 A 26.468 73.889 6.287 52 С PRO A 79 40 MOTA 1.00 29.57 A 6.377 26.391 75.108 79 53 0 PRO A MOTA 27.279 1.00 29.77 A 73.268 5.435 N GLU A 80 MOTA 54 1.00 29.55 A 4.533 28.179 73.975 55 CA GLU A 80 ATOM 1.00 32.88 A 29.043 72.980 3.768 GLU A 80 MOTA 56 CB 29.798 1.00 40.36 A 71.996 4.643 GLU A 80 57 CG 45 MOTA 5.367 28.879 1.00 44.21 A 71.014 58 CD GLU A 80 ATOM 28.000 1.00 46.94 A 70.422 4.700 59 OE1 GLU A 80 MOTA 1.00 45.47 A 70.828 6.598 29.038 OE2 GLU A 80 60 ATOM 1.00 28.32 A 27.479 74.872 3.524 61 C GLU A 80 MOTA 28.126 1.00 28.20 A 2.894 75.709 62 0 GLU A 80 50 MOTA 1.00 26.28 A 26.168 3.342 74.698 N ASP A 81 MOTA 63 1.00 23.59 A 75.528 2.384 25.441 6.4 CA ASP A 81 **ATOM** 1.00 25.08 A 24.184 74.834 1.888 CB ASP A 81 65 MOTA 1.00 28.14 A 24.477 73.510 1.225 66 CG ASP A 81 MOTA 1.00 29.12 A 73.369 0.625 25.578 67 OD1 ASP A 81 55 ATOM 1.00 28.33 A 72.617 1.294 23.601 OD2 ASP A 68 81 MOTA 1.00 23.24 A 76.856 2.967 25.046 C ASP A 81 69 ATOM 1.00 24.29 A 24.519 77.716 2.257 70 0 ASP A 81 ATOM 25.309 1.00 21.34 A 77.036 4.259 N PHE A 82

1.00 20.86 A ATOM . 72 CA PHE A 82 78.272 4.930 24.946 77.992 6.029 23.929 1.00 18.34 A ATOM CB PHE A 82 73 1.00 19.18 A 22.683 ATOM 74 CG PHE A 82 77.355 5.536 CD1 PHE A 5.099 21.610 1.00 19.28 A 82 78.138 ATOM 75 CD2 PHE A 82 75.974 5.462 22.588 1.00 17.82 A 76 ATOM 1.00 17.94 A PHE A 82 77.551 4.597 20.461 ATOM 77 CE1 PHE A 75.371 4.961 21.449 1.00 19.08 A MOTA 78 CE₂ 82 1.00 20.45 A CZPHE A 82 76.164 4.525 20.376 ATOM 79 26.105 1.00 21.71 A 80 С PHE A 82 78.982 5.555 MOTA 78.418 27.173 1.00 24.82 A 5.739 10 PHE A 82 ATOM 81 0 LYS A 80.244 5.865 25.869 1.00 21.83 A N 83 MOTA 82 CA LYS A 83 81.077 6.555 26.823 1.00 22.27 A ATOM 83 1.00 24.03 A 27.148 MOTA 84 CB LYS A 83 82.327 5.750 83.074 28.340 1.00 30.99 A LYS A 6.320 85 CG 83 MOTA 6.827 27.993 84.465 1.00 35.16 A 15 CD LYS A 83 MOTA .86 27.945 1.00 39.06 A LYS A 83 85.465 5.683 87 CE ATOM 85.512 4.974 29.266 1.00 41.00 A 88 ΝZ LYS A 83 ATOM 25.998 1.00 22.51 A ATOM 89 C LYS Α 83 81.462 7.775 25.120 1.00 23.24 A 7.677 82.324 MOTA 90 0 LYS Α 83 80.800 8.907 26.227 1.00 20.27 A 20 PHE A 84 MOTA 91 N 10.098 25.454 1.00 19.31 A CA PHE A 84 81.118 92 MOTA 25.605 1.00 19.95 A 80.016 11.145 93 CB PHE A 84 MOTA 10.694 25.075 1.00 20.81 A PHE A 84 78.683 MOTA 94 CG 25.835 1.00 21.62 A MOTA 95 CD1 PHE A 84 77.855 9.879 23.804 1.00 20.47 A 78.278 11.035 CD2 PHE A 84 25 MOTA 96 76.665 9.418 25.339 1.00 19.26 A 97 CE1 PHE A 84 MOTA 23.300 1.00 18.97 A MOTA 98 CE2 PHE A 84 77.073 10.568 9.764 24.068 1.00 19.78 A 76.276 MOTA 99 ·CZ PHE A 84 82.463 10.680 25.863 1.00 19.58 A C PHE A 84 MOTA 100 82.888 10.540 26.998 1.00 20.60 A 0 PHE A 84 30 ATOM 101 1.00 19.33 A 24.913 83.141 11.307 N GLY A 85 MOTA 102 25.169 1.00 18.23 A 84.434 11.909 GLY A 85 MOTA 103 CA 84.480 13.368 24.743 1.00 19.96 A MOTA 104 C GLY A 85 24.962 1.00 20.02 A GLY A 83.533 14.124 105 O 85 MOTA 1.00 20.79 A 85.568 13.764 24.101 N LYS A 86 35 MOTA 106 23.704 1.00 22.45 A MOTA 107 CA LYS A 86 85.736 15.159 15.400 23.210 1.00 22.06 A 87.168 ATOM 108 CB LYS A 86 1.00 23.37 A 87.399 15.048 21.751 MOTA 109 CG LYS A 86 1.00 26.45 A 88.832 14.591 21.505 ATOM 110 CD LYS A 86 1.00 30.25 A 15.275 20.294 89.451 40 MOTA 111 CE LYS A 86 16.721 20.553 1.00 33.08 A 89.771 112 NZ LYS A 86 MOTA 1.00 21.50 A 84.750 15.668 22.661 MOTA 113 С LYS A 86 14.900 21.916 1.00 21.98 A 84.154 O LYS A 86 **ATOM** 114 1.00 20.15 A 115 N ILE A . 87 84.582 16.985 22.647 MOTA 21.705 1.00 19.38 A 17.661 45 MOTA 116 CA ILE A 87 83.712 22.272 1.00 17.37 A 83.270 19.037 MOTA 117 CB ILE A 87 1.00 15.07 A 82.724 19.935 21.163 MOTA 118 CG2 ILE A 87 82.222 18.800 23.371 ·1.00 18.62 A ATOM 119 CG1 ILE A 87 1.00 16.91 A 24.190 81.848 20.025 MOTA 120 CD1 ILE A 87 17.836 20.436 1.00 19.85 A 50 121 C ILE A 87 84.549 MOTA 20.502 1.00 21.66 A 85.666 18.317 MOTA 122 0 ILE A 87 84.030 17.406 19.293 1.00 19.65 A 123 N LEU A ATOM 88 1.00 20.20 A 18.047 MOTA 124 CA LEU A 88 84.771 17.539 17.078 1.00 18.76 A MOTA 84.423 16.405 125 CB LEU A 88 84.807 14.981 17.493 1.00 16.99 A 55 ATOM 126 CG LEU A 88 1.00 13.92 A 16.570 ATOM 127 CD1 LEU A 88 84.122 13.995 1.00 11.51 A 86.305 14.809 17.441 128 CD2 LEU A 88 ATOM 1.00 20.87 A 84.429 18.861 17.407 129 C MOTA LEU A 88 85.233 19.443 16.709 1.00 21.48 A MOTA 130 0 LEU A 88

	•									
	MOTA	131	N	GLY :		89	83.221		17.639	1.00 22.34 A
	MOTA	132	CA	GLY .		89	82.856	20.601	17.043	1.00 25.87 A
	ATOM	133	C	GLY .	A	89	81.476	21.057	17.451	1.00 29.45 A
	ATOM	134	0	GLY .	A	89	80.673	20.292	17.990	1.00 29.48 A
5	ATOM	135	N	GLU .	A	90	81.196	22.321	17.188	1.00 32.71 A
	ATOM	136	CA	GLU .	A	90	79.904	22.864	17.530	1.00 37.61 A
	MOTA	137	CB	GLU .	A	90	80.047	23.798	18.738	1.00 38.05 A
	ATOM	138	CG	GLU .	A	90	80.123	22.998	20.037	1.00 42.04 A
	ATOM	139	CD	GLU .	A	90	80.463	23.813	21.270	1.00 45.47 A
10	ATOM	140	OE1	GLU .	Α	90	81.662	24.137	21.477	1.00 47.26 A
	ATOM	141	OE2	GLU .	Α	90	79.524	24.119	22.041	1.00 47.39 A
	MOTA	142	С	GLU	A	90	79.277	23.565	16.349	1.00 40.01 A
	MOTA	143	0	GLU	A	90	79.972	24.148	15.518	1.00 42.05 A
	ATOM	144	N	GLY	A	91	77.962	23.440	16.240	1.00 42.05 A
15	ATOM	145	CA	GLY	Α	91	77.238	24.102	15.174	1.00 43.15 A
	ATOM	146	С	GLY	A	91	76.276	25.035	15.892	1.00 45.06 A
	ATOM	147	0	GLY	Α	91	76.317	25.149	17.134	1.00 43.58 A
	ATOM	148	N	SER	Α	92	75.408	25.699	15.136	1.00 46.66 A
	ATOM	149	CA	SER	Α	92	74.430	26.606	15.742	1.00 48.21 A
20	ATOM	150	CB	SER	Α	92	73.754	27.462	14.660	1.00 51.13 A
	ATOM	151	OG	SER	Α	92	73.601	26.741	13.439	1.00 54.79 A
	ATOM	152	C	SER	A	92	73.382	25.827	16.538	1.00 47.10 A
	MOTA	153	0	SER	A	92	73.055	26.190	17.678	1.00 49.44 A
	MOTA	154	N	PHE	Α	93	72.874	24.743	15.957	1.00 44.39 A
25	ATOM	155	CA	PHE	A	93	71.866	23.942	16.648	1.00 41.99 A
	ATOM	156	CB.	PHE	Α ·	93	70.617	23.798	15.780	1.00 43.92 A
	ATOM	157	CG	PHE	Α	93	70.434	24.919	14.814	1.00 47.66 A
	ATOM	158	CD1	PHE	A	93	70.689	24.729	13.455	1.00 49.35 A
	ATOM	159	CD2	PHE	Α	93	70.061	26.185	15.264	1.00 49.16 A
30	ATOM	160	CE1	PHE	Α	93	70.581	25.789	12.551	1.00 51.11 A
	ATOM	161	CE2			93	69.949	27.257	14.374	1.00 50.58 A
	ATOM	162	CZ	PHE	Α	93	70.209	27.062	13.014	1.00 51.37 A
	MOTA	163	С	PHE	Α	93	72.352	22.555	17.028	1.00 38.35 A
	MOTA	164	0	PHE	А	93	71.532	21.670	17.257	1.00 38.33 A
35	MOTA	165	N	SER	A	94	73.665	22.351	17.106	1.00 33.28 A
	MOTA	166	CA	SER	Α	94	74.151	21.028	17.440	1.00 29.57 A
	ATOM	167		SER		94	73.996	20.106	16.227	1.00 30.45 A
	MOTA	168	OG	SER	Α	94	75.123	20.190	15.368	1.00 30.51 A
	MOTA	169	Ċ	SER		94	75.588	20.952	17.936	1.00 27.66 A
40	MOTA	170	0	SER		94	76.369	21.893	17.803	1.00 27.25 A
	ATOM	171	N	THR		95	75.927	19.807	18.512	1.00 25.06 A
	MOTA	172	CA	THR		95	77.264	19.572	19.027	1.00 23.70 A 1.00 24.12 A
	ATOM	173	CB	THR		95	77.310	19.626	20.582	1.00 24.12 A 1.00 25.68 A
	MOTA	174	OG1			95	76.801	20.886	21.044	1.00 23.00 A 1.00 22.92 A
45	MOTA	175	CG2			95	78.731	19.458	21.073	1.00 22.92 A 1.00 22.05 A
	MOTA	176	С	THR		95	77.655	18.180	18.594	1.00 22.03 A 1.00 21.43 A
	ATOM	177	0	THR		95	76.860	17.250	18.673	1.00 21.43 A
•	MOTA	178	N	VAL		96	78.883	18.029	18.129	1.00 21.52 A 1.00 19.53 A
	MOTA	179	CA	VAL		96	79.348	16.723	17.702	1.00 19.33 A
50	MOTA	180	CB	VAL		96	79.980	16.818	16.316	1.00 17.73 A
	MOTA	181		VAL		96	80.418	15.443	15.839	1.00 17.73 A
	MOTA	1,82	•	VAL		96	78.983	17.442	15.353	1.00 18.03 A 1.00 19.43 A
	ATOM	183	C	VAL		96	80.364	16.242	18.722	1.00 19.43 A 1.00 19.84 A
	ATOM	184	0	VAL		96	81.372	16.910	18.959 19.324	1.00 17.90 A
55	ATOM	185	N	VAL		97	80.099	15.082		1.00 17.30 A
	ATOM	186	CA	VAL		97	80.989	14.532	20.341 21.736	1.00 17.32 A
	ATOM	187	CB	VAL		97 97	80.283 79.581	14.438 15.750	22.066	1.00 20.10 A
	ATOM	188		LAV		97 97	79.381	13.750	21.713	1.00 23.78 A
	MOTA	189	CG2	VAL	A	97	13.234	13.33/	21.113	

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	MOTA	190	C	VAL	A	97	81.471	13.144	19.949	1.00 17.15 A
	ATOM	191	0	VAL	Α	97	80.727	12.351	19.379	1.00 18.17 A
	ATOM	192	N	LEU	Α	98	82.735	12.866	20.243	1.00 17.34 A
	MOTA	193	CA	LEU	A	98	83.331	11.575	19.974	1.00 17.44 A
5	ATOM	194	CB	LEU	Α	98	84.853	11.689	19.990	1.00 17.84 A
	ATOM	195	CĢ	LEU	Α	98	85.656	10.407	19.737	1.00 18.59 A
	MOTA	196	CD1	LEU	A	98	85.259	9.803	18.387	1.00 18.87 A
	MOTA	197	CD2	LEU	Α	98	87.151	10.738	19.772	1.00 16.62 A
	MOTA	198	C	LEU	A	98	82.874	10.626	21.081	1.00 18.35 A
10	MOTA	199	0	LEU	Α	98	82.992	10.926	22.259	1.00 18.60 A
	MOTA	200	N	ALA	Α	99	82.340	9.476	20.697	1.00 19.15 A
	MOTA	201	CA	ALA	Α	99	81.888	8.513	21.675	1.00 19.73 A
	MOTA	202	CB	ALA	A	99	80.383	8.534	21.759	1.00 17.97 A
	MOTA	203	C	ALA	A	99	82.360	7.117	21.317	1.00 21.86 A
15	MOTA	204	0	ALA	A	99	82.502	6.766	20.131	1.00 22.18 A
-	MOTA	205	N	ARG	Α	100	82.631	6.324	22.345	1.00 21.93 A
	ATOM	206	CA	ARG	A	100	83.025	4.963	22.102	1.00 23.29 A
	ATOM	207	CB	ARG	A	100	84.333	4.637	22.805	1.00 25.99 A
	MOTA	208	CG	ARG	Α	100	84.870	3.271	22.388	1.00 31.56 A
20	ATOM	209	CD	ARG	Α	100	86.146	2.923	23.129	1.00 35.19 A
	ATOM	210	NE	ARG	Α	100	87.220	3.875	22.847	1.00 37.39 A
	MOTA	211	CZ	ARG	Α	100	87.958	3.870	21.740	1.00 38.05 A
	MOTA	212	NH1	ARG	Α	100	87.742	2.953	20.797	1.00 37.25 A
	MOTA	213		ARG	A	100	88.918	4.780	21.580	1.00 36.22 A
25	MOTA	214	,C			100	81.904	4.060	22.603	1.00 22.07 A
	MOTA	215	0			100	81.460	4.177	23.743	1.00 22.10 A
	ATOM	216	N			101	81.417	3.189		1.00 21.29 A
	ATOM	217	CA			101	80.357	2.262	22.119	1.00 22.87 A
	MOTA	218	CB			101	79.747	1.631	20.867	1.00 23.10 A
30	ATOM	219	CG			101	78.740	0.563	21.148	1.00 22.71 A
	ATOM	220	CD			101	78.128	0.040	19.878	1.00 23.56 A
	ATOM	221		GLU			78.892	-0.198	18.922	1.00 21.84 A
	ATOM	222		GLU			76.890	-0.143	19.832	1.00 26.29 A
	ATOM	223	C			101	80.942	1.176	23.037	1.00 21.56 A
35	ATOM	224	0			101	81.884	0.485	22.666	1.00 20.69 A 1.00 21.11 A
	ATOM	225	N			102	8,0.389	1.042	24.236	1.00 21.11 A
	MOTA	226	CA			102	80.874	0.057	25.204	1.00 21.34 A
	ATOM	227	CB			102	80.075	0.199	26.507	1.00 20.30 A 1.00 22.35 A
40	ATOM		CG			102	80.193	1.620 1.798	27.092 28.207	1.00 20.18 A
40	ATOM	229		LEU		102	79.177 81.600	1.756	27.608	1.00 20.10 A
	ATOM	230	CD2			102	80.896	-1.415	24.729	1.00 20.27 A
	ATOM ATOM	231	С 0			102	81.922	-2.078	24.725	1.00 21.63 A
		232 233	N			102	79.792	-1.922	24.201	1.00 18.37 A
15	ATOM				_			-3.307	23.731	1.00 20.54 A
45	ATOM ATOM	234 235	CA CB			103	78.333	-3.694	23.359	1.00 19.31 A
	ATOM	235	CP			103		-3.658	22.552	1.00 22.26 A
	ATOM	237	0			103	81.002	-4.829	22.358	1.00 23.93 A
	ATOM	237	N			104	81.141	-2.677	21.775	1.00 20.79 A
50	ATOM	239	CA			104		-2.999	20.622	1.00 21.40 A
20	ATOM	240	CB			104	81.279	-2.632	19.326	1.00 20.97 A
	MOTA	241		THR			81.174	-1.205	19.259	1.00 23.21 A
	ATOM	242	CG2			104	79.891	-3.266	19.245	1.00 19.82 A
	ATOM	243	C			104	83.304	-2.300	20.569	1.00 23.57 A
55	ATOM	244	o			104	84.168	-2.687	19.796	1.00 23.41 A
-	ATOM	245		SER			83.454	-1.243	21.359	1.00 24.64 A
	ATOM	246	CA			105		-0.487	21.390	1.00 24.23 A
	ATOM	247	CB			105		-1.467	21.481	1.00 25.40 A
	ATOM	248	OG			105			21.719	1.00 34.15 A

	MOTA	249	С	SER A	A 105	84.819	0.454	20.163	1.00 23.42 A
	MOTA	250	0	SER A	A 105	85.803	1.187	20.013	1.00 23.28 A
	ATOM	251	N	ARG A	A 106	83.821	0.448	19.295	1.00 21.19 A
	MOTA	252	CA	ARG I	A 106	83.850	1.323	18.115	1.00 22.25 A
5	ATOM	253	CB	ARG A	A 106	82.754	0.922	17.118	1.00 24.82 A
	ATOM	254	CG		A 106	83.027	-0.343	16.349	1.00 25.20 A
	ATOM	255	CD	ARG A	A 106	81.740	-0.942	15.884	1.00 25.19 A
	MOTA	256	NE	ARG A	A 106	81.972	-1.900	14.815	1.00 26.11 A
	MOTA	257	CZ		A 106	81.042	-2.707	14.322	1.00 24.24 A
10	MOTA	258	NH1	ARG 2	A 106	79.805	-2.677	14.818	1.00 21.06 A
	ATOM	259		ARG 2		81.351	-3.513	13.315	1.00 20.25 A
	ATOM	260	C	ARG .	A 106	83.655	2.806	18.433	1.00 19.79 A
	ATOM	261	0		A 106	82.836	3.175	19.266	1.00 18.73 A
	ATOM	262	N	GLU .	A 107	84.404	3.646	17.736	1.00 19.82 A
15	MOTA	263	CA	GLU .	A 107	84.294	5.086	17.903	1.00 21.14 A
	MOTA	264	CB	GLU .	A 107	85.656	5.746	17.777	1.00 21.88 A
	MOTA	265	CG	GLU .	A 107	86.562	5.428	18.926	1.00 26.09 A
	MOTA	266	CD	GLU .	A 107	87.916	6.043	18.746	1.00 30.29 A
	MOTA	267	OE1	GLU .	A 107	88.212	7.057	19.434	1.00 32.48 A
20	MOTA	268	OE2	GLU .	A 107	88.678	5.512	17.901	1.00 31.98 A
	MOTA	269	C	GLU .	A 107	83.358	5.693	16.870	1.00 20.50 A
	ATOM	270	.0	GLU	A 107	83.474	5.429	15.676	1.00 20.70 A
	MOTA	271	N	TYR	A 108	82.415	6.498	17.347	1.00 20.38 A
	ATOM	272	CA	TYR	A 108	81.464	7.172	16.477	1.00 18.49 A
25	ATOM	273	CB	TYR	A 108	80.049	6.660	16.700	1.00 17.92 A
	ATOM .	274	CG	TYR	A 108	79.828	5.247	16.238	1.00 23.37 A
	MOTA	275			A 108	79.598	4.964	14.886	1.00 22.79 A
	MOTA	276	CE1	TYR	A 108	79.357	3.648	14.458	1.00 23.56 A
•	MOTA	277	CD2	TYR	A 108	79.820	4.180	17.154	1.00 21.34 A
30	MOTA	278	CE2		A 108	79.583	2.873	16.740	1.00 20.43 A
	MOTA	279	CZ		A 108	79.346	2.609	15.392	1.00 23.44 A
	MOTA	280	OH		A 108	79.061	1.321	14.972	1.00 24.10 A
	MOTA	281	С		A 108	81.478	8.635	16.828	1.00 18.53 A
,	MOTA	282	Ο,		A 108	81.778		17.971	1.00 17.37 A
35	MOTA	283	N		A 109	81.169	9.453	15.829	1.00 17.24 A
	MOTA	284	CA		A 109	81.053	10.885	16.006	1.00 15.98 A
	MOTA	285	CB		A 109	81.597	11.600	14.788	1.00 15.20 A
	ATOM	286	C		A 109	79.528	11.087	16.140	1.00 15.73 A 1.00 15.79 A
'	MOTA	287	0		A 109	78.767	10.873	15.191	1.00 15.75 A
40	MOTA	288	N		A 110	79.070	11.474	17.320	1.00 14.95 A 1.00 15.99 A
	MOTA	289	CA		A 110	77.636	11.636	17.511	1.00 15.55 A
	MOTA	290	CB		A 110	77.188	10.940 11.126	18.815 19.039	1.00 13.31 A
	MOTA	291	CG2		A 110	75.697		18.729	1.00 14.44 A
	ATOM	292	CG1		A 110	77.541	9.452		
45	MOTA	293			A 110	76.964	8.595	19.847 17.514	1:00 16.83 A 1.00 16.55 A
	MOTA	294	C		A 110	77.176	13.085	18.370	1.00 16.33 A
	MOTA	295	0		A 110	77.583	13.873	16.538	1.00 16.24 A
	ATOM	296	N		A 111	76.343	13.430	16.430	1.00 18.03 A
	ATOM	297	CA		A 111	75.804	14.777	14.997	1.00 18.21 A 1.00 19.36 A
50	ATOM	298	CB		A 111		15.065 16.548	14.768	1.00 19.38 A
	ATOM	299	CG		A 111	75.035		13.396	1.00 22.00 A 1.00 23.67 A
	MOTA	300	CD		A 111		16.844 18.222	12.930	1.00 23.07 A
	ATOM	301	CE		A 111				1.00 28.83 A
٠.	ATOM	302	NZ		A 111		18.938 14.866	17.383	1.00 20.03 A
55	ATOM	303	C		A 111			17.239	1.00 18.27 A
	MOTA	304	0		A 111			18.344	1.00 15.41 A
	ATOM	305	N		A 112 A 112			19.331	1.00 16.56 A
	ATOM	306	CA		A 112			20.777	1.00 17.09 A
	MOTA	307	CB	TUE	~ 114	・/ せ・エブせ	40.047		

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	MOTA	308	CG2	ILE	A	112		73.073	15.926	21.830	1.00	11:60 7	A
	MOTA	: 309	CG1	ILE	A	112		74.957	14.480	20.885	1.00	16.81 7	Ą
	MOTA	310	CD1	ILE	Α	112		75.771	14.262	22.178	1.00	15.96 A	A
	MOTA	311	C	ILE	Α	112		72.876	17.261	19.158	1.00	17.98 7	A.
5	ATOM	312	0	ILE	A	112		73.504	18.314	18.965	1.00	16.70 2	4
	MOTA	313	N	LEU	Α	113		71.546	17.198	19.195	1.00	19.61	A
	MOTA	314	CA	LEU	A	113		70.711	18.393	19.034	1.00	21.99 2	Ą
	MOTA	315	CB	LEU	A	113		70.058	18.434	17.641		22.17 1	
	MOTA	316	CG	LEU	Α	113		70.906	18.273	16.367		22.83	
10	ATOM	317	CD1	LEU	Α	113		71.124	16.792	16.059	1.00	22.72	A.
	MOTA	318	CD2	LEU	Α	113		70.191	18.912	15.206		21.97	
	MOTA	319	C ·	LEU	A	113		69.612	18.419	20.088		24.22	
	MOTA	320	0	LEU				69.062	17.378	20.469		24.61	
	MOTA	321	N	GLU	Α	114		69.285	19.615	20.559		27.06 7	
15	ATOM	322	CA	GLU	А	114		68.247	19.759	21.567		28.93	
-	MOTA	323	CB	GLU				68.586	20.926	22.488		31.39	
	MOTA	324	CG	GLU	Α	114		67.671	21.026			39.92	
	MOTA	325	CD	GLU	A	114		67.676	22.406	24.300		45.42	
	ATOM	326	OE1	GLU				67.160	23.356	23.655		46.90	
20	ATOM	327	OE2	GLU				68.204	22.540	25.429		50.09	
	ATOM	328	C	GLU				66.887	19.978	20.892		29.21	
	MOTA	329	0	GLU				66.679	20.969	20.177		29.53	
	MOTA	330	И	LYS				65.962	19.051	21.116		28.74	
-	ATOM	331	CA	LYS				64.642	19.152	20.507		29.44	
25	ATOM	332	CB.	LYS				63.744	18.002	20.987		28.12	
	ATOM	333	CG	LYS				63.827	16.758	20.103		28.47	
	ATOM	334	CD	LYS			,	63.026	15.571	20.639		27.07	
	MOTA	335	CE	LYS				63.738	14.854	21.779		28.88	
	MOTA	336	NZ	LYS				62.963	13.672	22.282			
30	MOTA	337	C	LYS				63.947	20.502	20.724		29.72 3 30.03	
	ATOM	338 -	0	LYS.				63.310	21.025	19.799		28.83	
	ATOM	339	N	ALA				64.082	21.091	21.910		29.91	
	ATOM	340	CA.	ALA				63.407	22.365 22.749	22.159 23.647		28.16	
25	ATOM	341	CB	ALA				63.470	23.480	21.311		30.93	
35	MOTA	342	C	ALA				63.976	24.217	20.667		32.28.	
	MOTA	343	0	ALA				63.231 65.297	23.593	21.292		31.66	
	ATOM	344	N CA	HIS HIS				65.951	24.645	20.523		32.13	
	MOTA	345		HIS				67.472	24.571	20.728		34.12	
40	ATOM	346	CB CG			117		68.219	25.741	20.169		37.74	
40	ATOM ATOM	347 348		HIS				67.794	26.959	19.761		39.67	
	ATOM	349		HIS				69.582	25.727	19.966		42.04	
	ATOM	350		HIS				69.965	26.884	19.454		41.07	
	ATOM	351		HIS				68.899	27.649	19.320		40.56	
45		352	C	HIS				65.600	24.547	19.040		31.36	
45	ATOM ATOM	353	o			117		65.466	25.560	18.350		32.37	
	ATOM	354	N			118		65.430	23.330	18.544		30.26	
	ATOM	355	CA			118		65.102	23.158	17.132		29.28	
	ATOM	356	CB			118	•	65.266	21.696	16.712		27.64	
50	ATOM	357	CG2			118		64.560		15.401		22.46	
50	MOTA	358		ILE				66.756	21.371	16.642		27.22	
	ATOM	359	_	ILE				67.036	19.917	16.437		30.51	
	ATOM	360	C			118		63.688	23.618	16.816		30.41	
	ATOM	361	ō			118		63.444	24.251	15.785		29.55	
55 ·	ATOM	362	N			119		62.756	23.291	17.705	1.00	29.59	А
	ATOM	363	CA			119		61.376	23.682	17.497		29.18	
	ATOM	364	CB			119		60.447	22.979	18.506	1.00	27.15	A
	ATOM	365		ILE	A	119		59.071	23.623	18.486		22.69	
	ATOM	366		ILE				60.394	21.486	18.173	1.00	23.45	A

	ATOM	367	CD1	ILE A	. 119	59.666	20.665	19.173	1.00 19.08 A
	ATOM	368	С	ILE A	119	61.223	25.194	17.617	1.00 30.65 A
	ATOM	369	0	ILE A	119	60.574	25.832	16.786	1.00 30.59 A
	ATOM	370	N	ALA A	120	61.837	25.768	18.642	1.00 31.95 A
5	ATOM	371	CA	ALA A	120	61.752	27.205	18.848	1.00 33.69 A
	ATOM	372	CB '	ALA A	120	62.473	27.608	20.150	1.00 33.17 A
	ATOM	373	C	ALA A	120	62.330	27.973	17.671	1.00 34.80 A
	ATOM	374	0	ALA A	120	61.865	29.067	17.362	1.00 37.34 A
	ATOM	375	N	GLU F	121	63.328	27.413	16.997	1.00 35.09 A
10	ATOM	376	CA	GLU F	121	63.941	28.116	15.872	1.00 35.31 A
	ATOM	377	CB	GLU F	121	65.453	27.927	15.933	1.00 39.72 A
	MOTA	378	CG	GLU A	121	66.103	28.735	17.038	1.00 45.91 A
	ATOM	379	CD	GLU A	121	65.955	30.225	16.784	1.00 49.51 A
	MOTA	380	OE1	GLU A	121	66.634	30.736	15.866	1.00 52.87 A
15	ATOM	381	OE2	GLU A	121	65.148	30.879	17.482	1.00 51.35 A
	MOTA	382	С	GLU A	121	63.421	27.699	14.499	1.00 34.14 A
	ATOM	383	0	GLU A	121	63.964	28.109	13.468	1.00 31.41 A
	MOTA	384	N	ASN A	122	62.363	26.891	14.497	1.00 33.86 A
	ATOM	385	CA	ASN A	122	61.771	26.367	13.266	1.00 34.00 A
20	ATOM	386	CB	ASN A	122,	61.112	27.473	12.464	1.00 36.75 A
	ATOM	387	CG	ASN A	122	59.962	28.081	13.193	1.00 39.62 A
	ATOM	388	OD1	ASN A	A 122	60.148	28.788	14.185	1.00 39.90 A
	ATOM	389	ND2	ASN A	A 122	58.753	27.794	12.727	1.00 41.02 A
	ATOM	390	C	ASN Z	A 122	62.798	25.686	12.397	1.00 31.78 A
25	ATOM	391	0	ASN Z	A 122	62.958	26.035	11.230	1.00 32.05 A
	ATOM	392	N	LYS Z	A 123	63.494	24.714	12.965	1.00° 28:71 A
	ATOM	393	CA	LYS 2	A 123	64.508	24.008	12.217	1.00 29.39 A
	ATOM	394	CB	LYS 2	A 123	65.842	24.036	12.974	1.00 31.70 A
	ATOM	395	. CG	LYS 3	A 123	66.434	25.416	13.132	1.00 33.49 A
30	MOTA	396	CD	LYS 3	A 123	66.612	26.076	11.763	1.00 37.43 A
	MOTA	397	CE	LYS 2	A 123	67.174	27.491	11.898	1.00 38.52 A
	ATOM	398	NZ	LYS 2	A 123	67.337	28.176	10.582	1.00 37.85 A
	MOTA	399	C '	LYS .	A 123	64.116	22.572	11.931	1.00 28.30 A
	ATOM	400	0	LYS .	A 123	64.867	21.844	11.289	1.00 29.68 A
35	MOTA	401	N	VAL .	A 124	62.944	22.162	12.404	1.00 26.80 A
	ATOM	402	CA	VAL .	A 124	62.484	20.796	12.175	1.00 26.73 A
	ATOM	403	CB	VAL .	A 124	61.024	20.593	12.622	1.00 26.31 A
•	MOTA	404	CG1	VAL	A 124	60.532	19.222	12.191	1.00 25.31 A
	MOTA	405	CG2	VAL	A 124	60.918	20.720	14.134	1.00 26.73 A
40	MOTA	406	С		A 124	62.594	20.351	10.722	1.00 27.11 A
	MOTA	407	0	VAL	A 124	62.973	19.218	10.450	1.00 29.79 A
	ATOM	408	N	PRO	A 125	62.270	21.228	9.763	1.00 27.28 A
	MOTA	409	CD.	PRO	A 125	61.610	22.544	9.818	1.00 27.49 A
	MOTA	410	CA		A 125	62.386	20.758	8.378	1.00 27.41 A
45	MOTA	411	CB	PRO	A 125	61.775	21.904	7.563	1.00 26.08 A
	MOTA	412	CG	PRO	A 125	60.821	22.546	8.524	1.00 27.54 A
	MOTA	413	C		A 125	63.837	20.506	8.006	1.00 27.90 A
	ATOM	414	0		A 125	64.162	19.572	7.260	1.00 26.27 A
	MOTA	415	N		A 126	64.703	21.350	8.550	1.00 28.64 A
50	MOTA	416	CA		A 126		21.271	8.288	1.00 30.11 A
	MOTA	417	CB		A 126	66.791	22.528	8.809	1.00 36.70 A
	MOTA	418	CG		A 126	66.440	23.774	8.013	1.00 44.64 A
	ATOM	419			A 126	66.984	23.988	6.744	1.00 47.43 A
	MOTA	420			A 126	66.737	25.173	6.037	1.00 50.16 A
55	MOTA	421			A 126	65.620	24.774	8.557	1.00 47.03 A
	MOTA	422	CE2		A 126	65.369	25.955	7:861	1.00 49.52 A 1.00 50.60 A
	ATOM	423	CZ		A 126	65.936	26.152	6.605	1.00 50.60 A 1.00 52.77 A
	MOTA	424	OH		A 126	65.754			
	MOTIZ	425	C	TYR	A 126	66.794	20.041	8.874	1.00 28.69 A

	ATOM	426	0	TYR	Α	126	67.613	19.407	8.208	1.00 28.32 A
	MOTA	427	N	VAL	A	127	66.464	19.714	10.118	1.00 25.64 A
	ATOM	428	CA	VAL	A	127	67.033	18.550	10.766	1.00 24.89 A
-	ATOM	429	CB	VAL	А	127	66.664	18.513	12.258	1.00 26.70 A
5	ATOM	430	CG1	VAL			67.158	17.206	12.881	1.00 22.51 A
	ATOM	431		VAL			67.255	19.743	12.972	1.00 23.84 A
	ATOM	432	C	VAL			66.521	17.276	10.097	1.00 24.81 A
•	ATOM	433	ŏ	VAL			67.260	16.315	9.890	1.00 24.02 A
	ATOM	434	N	THR			65.245	17.290	9.755	1.00 24.02 A
10	ATOM	435	CA	THR			64.608	16.164	9.088	1.00 24.59 A
	ATOM	436	CB	THR			63.123	16.471	8.843	1.00 25.38 A
	ATOM	437	OG1				62.478	16.652	10.106	1.00 25.76 A
	ATOM	438	CG2				62.451	15.354	8.066	1.00 23.70 A
	ATOM	439	C	THR			65.266	15.875	7.744	1.00 24.53 A
15	ATOM	440	ō	THR			65.560	14.729	7.426	1.00 25.53 A
	ATOM	441	И	ARG			65.477	16.925	6.957	1.00 23.33 A
	ATOM	442	CA	ARG			66.099	16.812	5.646	1.00 24.82 A 1.00 25.49 A
	ATOM	443	CB	ARG			66.111	18.181	4.959	1.00 25.49 A 1.00 26.78 A
	ATOM	444	CG	ARG			66.648	18.175		
20	ATOM	445	CD	ARG			66.579	19.563	3.529	1.00 32.33 A
20	ATOM	446	NE	ARG			65.326		2.878	1.00 36.93 A
-	ATOM	447	CZ	ARG				20.249	3.184	1.00 42.70 A
	ATOM	448					65.254	21.462	3.730	1.00 46.67 A
	ATOM	449		ARG ARG			66.366	22.128	4.018	1.00 48.50 A
25	ATOM		C	ARG			64.073	21.997	4.027	1.00 48.90 A
23	ATOM	450 451	0				67.532	16.296	5.801	1.00 26.46 A
	ATOM			ARG			68.002	15.456	5.020	1.00 24.76 A
		452	N	GLU			68.216	16.795	6.825	1.00 25.56 A
	ATOM	453	CA				69.582	16.393	7.076	1.00 28.29 A
20	ATOM	454	CB	GLU			70.118	17.106	8.310	1.00 27.95 A
30	ATOM	455	CG	GLU			71.591	16.875	8.539	1.00 29.48 A
	ATOM	456	CD	GLU			72.107	17.566	9.787	1.00 32.14 A
	ATOM	457		GLU			71.297	18.221	10.483	1.00 32.67 A
	ATOM	458		GLU			73.325	17.450	10.069	1.00 32.21 A
25	ATOM	459	C	GLU			69.665	14.886	7.279	1.00 29.86 A
35	ATOM	460	0	GLU			70.498	14.200	6.668	1.00 29.35 A
	ATOM	461	N	ARG			68.797	14.382	8.150	1.00 30.84 A
	ATOM	462	CA	ARG			68.763	12.966	8.451	1.00 31.62 A
	ATOM	463		ARG			67.786	12.684	9.598	1.00 33.12 A
40	ATOM	464	CG	ARG			67.557	11.190	9.831	1.00 36.17 A
40	ATOM	465	CD	ARG			66.560	10.925	10.946	1.00 41.69 A
	ATOM	466	NE	ARG			66.330	9.492	11.166	1.00 46.62 A
	ATOM	467	CZ	ARG			65.692	8.986	12.224	1.00 48.29 A
	ATOM	468		ARG			65.215	9.795	13.165	1.00 49.51 A
4.5	ATOM	469		ARG			65.544	7.671	12.352	1.00 48.76 A
45	ATOM		C	ARG			68.371	12.138	7.235	1.00 30.59 A
	ATOM	471	0 .	ARG			68.897	11.051	7.026	1.00 29.96 A
	ATOM	472	N	ASP			67.446	12.649	6.433	1.00 29.54 A
	MOTA	473	CA	ASP			67.000	11.913	5.259	1.00 29.40 A
- ·	MOTA	474	CB	ASP			65.735	12.565	4.708	1.00 32.43 A
50	MOTA	475	CG	ASP			64.531	12.395	5.655	1.00 38.15 A
	ATOM	476		ASP .			64.749	12.227		1.00 40.40 A
	MOTA	477		ASP			63.365	12.439	5.186	1.00 41.19 A
	ATOM	478	C	ASP			68.088	11.789	4.189	1.00 27.62 A
	ATOM	479	0	ASP			68.232	10.744	3.553	1.00 26.54 A
55	ATOM	480	N	VAL .			68.862	12.850	4.011	1.00 25.14 A
	ATOM	481	CA	VAL .			69.939	12.857	3.044	1.00 24.12 A
	MOTA	482	CB	VAL .			70.451	14.272	2.833	1.00 24.07 A
	ATOM	483		VAL .			71.802	14.247	2.143	1.00 23.77 A
	ATOM	484	CG2	VAL .	A	133	69.461	15.030	2.008	1.00 24.30 A

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	ATOM	485	C	VAL	A	133	71.099	11.975	3.504	1.00 24.97 A
	MOTA	486	. 0	VAL			71.672	11.221	2.712	1.00 24.95 A
	ATOM	487	N	MET			71.458	12.074	4.779	1.00 23.41 A
	ATOM	488	CA	MET			72.539	11.255	5.268	1.00 23.12 A
5	ATOM	489	CB	MET	A	134	72.932	,11.653	6.683	1.00 21.12 A
	ATOM	490	CG	MET			73.608	13.005	6.759	1.00 21.21 A
	ATOM	491	SD	MET			74.530	13.204	8.291	1.00 20.52 A
	MOTA	492	CE	MET	A	134	73.172	13.347	9.534	1.00 17.71 A
	MOTA	493	C	MET			72.163	9.783	5.237	1.00 24.75 A
10	ATOM	494	0	MET			73.027	8.918	5.039	1.00 25.73 A
	ATOM	495	N	SER			70.885	9.474	5.425	1.00 23.96 A.
	ATOM	496	CA	SER	Α	135	70.484	8.064	5.408	1.00 24.82 A
	ATOM	497	CB	SER			69.048	7.889	5.917	1.00 24.63 A
	MOTA	498	OG	SER			68.139	8.496		1.00 29.80 A
15	MOTA	499	С	SER			70.585	7.479	4.003	1.00 22.35 A
	ATOM	500	0	SER			70.534	6.274	3.829	1.00 21.60 A
	MOTA	501	N	ARG			70.729	8.335	3.004	1.00 21.91 A
	MOTA	502	CA	ARG			70.815	7.858	1.631	1.00 23.76 A
	MOTA	503	CB	ARG			69.988	8.762	0.714	1.00 25.55 A
20	ATOM	504	CG	ARG			68.500	8.782	1.069	1.00 31.38 A
	MOTA	505	CD	ARG			67.764	9.897	0.332	1.00 33.65 A
	ATOM	506	NE	ARG			68.024	9.809	-1.099	1.00 38.77 A
	ATOM	507	CZ			136	67.654	10.718	-1.996	1.00 41.27 A
	ATOM	508		ARG			66.988	11.806	-1.604	1.00 42.53 A
25	ATOM	509		ARG			67.971	10.544	-3.286	1.00 39.41 A
	ATOM	510	С	ARG			72.248	7.789	1.131	1.00 22.64 A
-	ATOM	511	0	ARG			72.520	7.268	0.052	1.00 22.43 A
	ATOM	512	N	LEU			73.168	8.318	1.919	1.00 22.66 A
20	ATOM	513	CA	LEU			74.568	8.307	1.535	1.00 22.60 A
30	ATOM	514	CB	LEU			75.348	9.375	2.308	1.00 20.28 A
	MOTA	515	CG	LEU			74.842	10.793	2.068	1.00 19.72 A 1.00 17.83 A
	ATOM	516		LEU			75.695	11.816	2.840 0.564	1.00 17.83 A 1.00 18.39 A
	ATOM	517		LEU			74.855	11.062 6.950	1.775	1.00 18.39 A 1.00 22.60 A
35	ATOM	518 519	C O	LEU			75.195 75.203		2.892	1.00 22.00 A 1.00 23.75 A
23	ATOM ATOM	520	N	ASP			75.723	6.371	0.710	1.00 23.73 A 1.00 22.09 A
	ATOM	521	CA	ASP			76.383	5.083	0.788	1.00 22.63 A
	ATOM	522	CB	ASP			75.419	3.988	0.730	1.00 25.16 A
	ATOM	523	CG	ASP			75.976	2.622	0.582	1.00 26.26 A
40	ATOM	524		ASP			76.658	2.480	1.611	1.00 27.29 A
	ATOM	525		ASP			75.740	1.708	-0.237	1.00 30.75 A
	ATOM	526	C	ASP			77.617	5.112	-0.124	1.00 20.82 A
	ATOM	527	ō	ASP			77.656	4.445	-1.155	1.00 22.94 A
	ATOM	528	N	HIS			78.612	5.902	0.250	1.00 16.77 A
45	ATOM	529	CA	HIS			79.813	6.050	-0.557	1.00 16.21 A
	ATOM	530	СВ	HIS			79.614	7.180	-1.583	1.00 15.30 A
	ATOM	531	CG	HIS			80.755	7.348	-2.534	1.00 16.37 A
	ATOM	532	CD2	HIS			80.853	7.087	-3.860	1.00 15.32 A
	ATOM	533	ND1	HIS	Α	139	81.998	7.802	-2.139	1.00 17.12 A
50	ATOM	534	CE1	HIS	Α	139	82.811	7.810	-3.184	1.00 15.92 A
	ATOM	535	NE2	HIS	А	139	82.140	7.380	-4.238	1.00 13.96 A
	MOTA	536	С	HIS			80.985	6.371	0.357	1.00 16.70 A
	ATOM	.537	0	HIS			80.848	7.116	1.317	1.00 16.89 A
	ATOM	538	N	PRO	A	140	82.164	5.823	0.056	1.00 16.94 A
55	ATOM	539	CD	PRO	A	140	82.508	4.991	-1.108	1.00 17.10 A
	ATOM	540	CA	PRO	A	140	83.334	6.079	0.895	1.00 17.98 A
	ATOM .	541	CB	PRO	Α	140	84.390	5.163	0.291	1.00 17.03 A
	ATOM	542	CG	PRO	A	140	84.003	5.114	-1.159	1.00 18.59 A
	MOTA	543	С	PRO	A	140	83.822	7.528	1.070	1.00 18.59 A

	ATOM	544	0	PRO	Α	140	84.528	7.817	2.021	1.00 20.11 A	
	ATOM	545	N	PHE	Α	141	83.460	8.444	0.179	1.00 19.62 A	
	ATOM	546	CA	PHE	Α	141	83.909	9.833	0.345	1.00 18.34 A	
	ATOM	547	CB	PHE	Α	141	84.223	10.474	-1.010	1.00 17.53 A	
5	ATOM	548	CG	PHE	Α	141	85.440	9.880	-1.694	1.00 17.38 A	
	ATOM	549	CD1	PHE	Α	141	86.450	9.275	-0.938	1.00 17.01 A	
	ATOM	550	CD2	PHE	Α	141	85.579	9.926	-3.081	1.00 15.76 A	
	ATOM	551	CE1	PHE	A	141	87.572	8.724	-1.550	1.00 16.13 A	
	ATOM	552	CE2	PHE	Α	141	86.707	9.375	-3.708	1.00 16.99 A	
10	ATOM	553	CZ	PHE	Α	141	87.705	8.772	-2.938	1.00 15.01 A	
	ATOM	554	С	PHE	Ά	141	82.893	10.680	1.095	1.00 18.14 A	
	ATOM	555	0	PHE	Α	141	83.012	11.896	1.144	1.00 20.74 A	
	ATOM	556	N	PHE			81.901	10.037	1.697	1.00 15.85 A	
	ATOM	557	CA	PHE	Α	142	80.887	10.761	2.444	1.00 15.95 A	
15	ATOM	558	СВ	PHE			79.558	10.757	1.690	1.00 15.20 A	
	ATOM	559		PHE			79.507	11.721	0.542	1.00 15.62 A	
	ATOM	560		PHE			79.295	13.086	0.768	1.00 14.51 A	
	ATOM	561		PHE			79.651	11.265	-0.771	1.00 12.05 A	
	ATOM	562		PHE			79.222	13.991	-0.291	1.00 13.97 A	
20	ATOM	563		PHE			79.582	12.157	-1.840	1.00 15.46 A	
20	ATOM	564	CZ	PHE			79.365	13.536	-1.601	1.00 14.89 A	
	ATOM	565	C	PHE			80.654	10.167	3.824	1.00 15.60 A	
~	ATOM	566	o	PHE			80.886	8.986	4.061	1.00 15.39 A	
	ATOM	567	N	VAL			80.182	11.001	4.733	1.00 15.87 A	
25	ATOM	568	CA	VAL			79.878	10.564	6.075	1.00 15.04 A	
23	ATOM	569	CB	VAL			79.304	11.727	6.905	1.00 15.26 A	
	ATOM	570		VAL			78.012	12.231	6.276	1.00 11.03 A	
	ATOM	571		VAL			79.100	11.296	8.350	1.00 14.40 A	
	ATOM	572	C	VAL			78.828	9.479	5.935	1.00 15.52 A	
30	ATOM	573	0	VAL			78.076	9.453	4.963	1.00 15.45 A	
50	ATOM		·N	LYS			78.794	8.580	6.907		
	ATOM	575	CA	LYS			77.848	7.482	6.933	1.00 17.45 A	
	ATOM	576	CB	LYS			78.625	6.150	6.895	1.00 18.05 A	
	ATOM	577	CG	LYS			77.963	4.967	7.596	1.00 24.34 A	
35	ATOM	578	CD	LYS			76.922	4.263	6.752	1.00 26.35 A	
33		579	CE	LYS			77.461	2.926	6.213	1.00 30.22 A	
	ATOM `	580	NZ	LYS			77.576	1.882	7.271	1.00 28.27 A	
	ATOM	581	C	LYS			77.024	7.626	8.222	1.00 20.27 H	
		582	0	LYS			77.565	7.913	9.284	1.00 16.92 A	
40	ATOM ATOM	583	N	LEU			75.711	7.458	8.116	1.00 10.32 A	
40		584	CA	LEU			74.836	7.549	9.274	1.00 18.13 A	
	ATOM						73.514	8.210	8.893	1.00 18.86 A	
	ATOM	585.	CB	LEU			72.612	8.850	9.964	1.00 10.00 A	
	ATOM	586 587	CG	LEU		,	72.012	8.607	9.582	1.00 20.13 A	
45	ATOM			LEU					11.331	1.00 17.86 A	
45	ATOM	588		LEU			72.900	8.311	9.689		
	ATOM	589	C	LEU			74.559	6.113	9.669 8.954	1.00 18.85 A	
	ATOM	590	0	LEU			73.905	5.379		1.00 20.15 A 1.00 18.09 A	
	MOTA	591	N	TYR			75.030	5.713	10.867	1.00 18.09 A 1.00 15.93 A	
~ 0	ATOM	592	CA	TYR			74.830	4.341	11.329		
50	MOTA	593	CB	TYR			76.013	3.871	12.154	1.00 14.52 A	
	ATOM	594	CG			146	77.295	3.776	11.390	1.00 13.98 A 1.00 15.01 A	
	ATOM	595		TYR			78.093	4.907	11.193	1.00 15.01 A	
	MOTA	596		TYR			79.329	4.815	10.548		
	ATOM	597		TYR			77.752	2.541	10.912	1.00 14.36 A	
55	ATOM	598		TYR			78.984	2.426	10.266	1.00 15.47 A	
	ATOM	599	CZ			146	79.770	3.566	10.090	1.00 15.70 A	
	MOTA	600	OH				80.999	3.473	9.491	1.00 16.29 A	
•	MOTA	601	C			146 .	73.591	4.135	12.154	1.00 16.74 A	
	ATOM	602	0	TYR	Α	146	73.004	3.050	12.132	1.00 17.63 A	

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	ATOM	603	N	PHE .	A	147	73.198	5.158	12.901	1.00 15.90 A
	ATOM	604	CA	PHE .	A	147	72.012	5.041	13.745	1.00 17.10 A
	ATOM	605	CB	PHE .	Α	147	72.265	4.057	14.932	1.00 14.80 A
	ATOM	606	CG	PHE	A	147	73.509	4.366	15.747	1.00 16.36 A
5	ATOM	607	CD1	PHE			73.526	5.427	16.657	1.00 15.38 A
-	ATOM	608		PHE			74.701	3.663	15.514	1.00 16.83 A
	ATOM	609		PHE			74.709	5.801	17.314	1.00 15.96 A
	ATOM	610		PHE			75.907	4.024	16.163	1.00 16.65 A
	ATOM	611	CZ	PHE			75.908	5.107	17.069	1.00 16.96 A
10 ·	ATOM	612	C	PHE			71.550	6.378	14.286	1.00 17.73 A
10	ATOM	613	0	PHE			72.225	7.399	14.145	1.00 18.47 A
	ATOM	614	И	THR			70.376	6.352	14.897	1.00 19.28 A
			CA	THR			69.801	7.529	15.532	1.00 19.50 A
	MOTA	615					68.846	8.308	14.597	1.00 19.24 A
1.5	ATOM	616	CB	THR			67.722	7.485	14.271	1.00 13.24 A
15	ATOM	617		THR				8.727	13.311	1.00 18.23 A
	ATOM	618		THR			69.563			1.00 18.53 A 1.00 19.68 A
	ATOM	619	C	THR			68.976	7.071	16.718 16.802	
	ATOM	620	0	THR			68.556	5.915		1.00 20.20 A
	MOTA	621	N .	PHE			68.765	7.975	17.653	1.00 20.20 A
20	ATOM	622	CA	PHE			67.926	7.687	18.797	1.00 20.34 A
	MOTA	623	CB	PHE			68.558	6.626	19.728	1.00 19.06 A
	ATOM	624	CG	PHE			69.932	6.961	20.216	1.00 18.27 A
	MOTA	625		PHE			70.114	7.745	21.357	1.00 19.90 A
	MOTA	626		PHE			71.049	6.467	19.559	1.00 19.21 A
25	MOTA	627	CE1	PHE			71.387	8.028	21.840	1.00 19.04 A
	MOTA	628	CE2	PHE	A	149	72.341	6.741	20.025	1.00 19.95 A
	MOTA	629	CZ	PHE	Α	149	72.513	7.520	21:167	1.00 21.19 A
	MOTA	630	. C	PHE			67.693	9.004	19.487	1.00 20.94 A
	ATOM	631	0	PHE	Α	149	68.192	10.035	19.042	1.00 17.91 A
30	ATOM	632	N	GLN	Α	150	66.888	8.988	20.539	
	MOTA	633	CA	GLN	Ά	150 .	66.609	10.212	21.279	1.00 29.09 A
	MOTA	634	CB	GLN	Α	150	65.518	11.039	20.571	1.00 29.07 A
	MOTA	635	CG	GLN	Α	150	64.194	10.322	20.309	1.00 31.07 A
	ATOM	636	CD	GLN	Α	150	63.150	11.227	19.609	1.00 32.52 A
35	MOTA	637	OE1	GLN	A	150	62.503	12.075	20.243	1.00 30.50 A
	ATOM	638	NE2	GLN	A	150	63.009	11.056	18.294	1.00 29.34 A
	MOTA	639	C	GLN	A	150	66.190	9.927	22.707	1.00 29.59 A
	MOTA	640	0	GLN	Α	150	65.738	8.832	23.018	1.00 30.34 A
	ATOM	641	N	ASP	Α	151	66.407	10.892	23.590	1.00 31.52 A
40	ATOM	642	CA	ASP	A	151	65.957	10.750	24.967	1.00 32.22 A
	ATOM	643	CB	ASP	Α	151	67.093	10.948	25.974	1.00 31.30 A
	ATOM	644	CG	ASP	Α	151	67.832	12.246	25.790	1.00 32.39 A
	ATOM .	645	OD1	ASP	Α	151	67.241	13.217	25.263	1.00 34.30 A
	ATOM	646	OD2	ASP	Α	151	69.011	12.290	26.195	1.00 32.02 A
45	ATOM	647	C	ASP			64.914	11.858	25.063	1.00 33.56 A
	ATOM	648	0	ASP			64.495	12.387	24.033	1.00 34.76 A
	ATOM	649	N	ASP			64.498	12.239	26.261	1.00 35.00 A
	ATOM	650	CA	ASP			63.462	13.268	26.369	1.00 36.72 A
	ATOM	651	СВ	ASP			63.053	13.465	27.830	1.00 38.27 A
50	ATOM	652	CG	ASP			62.237	12.312	28.351	1.00 42.45 A
50	ATOM	653		ASP			61.377	11.824	27.579	1.00 43.52 A
	MOTA	654		ASP			62.444	11.900	29.519	1.00 44.28 A
	ATOM		· C	ASP			63.758	14.627	25.759	1.00 36.47 A
	ATOM	656	0	ASP			62.857	15.289	25.242	1.00 36.12 A
55	ATOM	657	Ŋ			153	65.021	15.029	25.781	1.00 36.09 A
,,	ATOM	658	CA			153	65.358	16.343	25.292	1.00 35.16 A
	MOTA	659	CB			153	65.976	17.137	26.442	1.00 39.45 A
	ATOM	660	CĠ			153	65.486	16.714	27.830	1.00 45.94 A
,	MOTA	661	CD			153	66.383	15.652	28.468	1.00 51.78 A
	117.01.1	001	CD.	250	• •					

	ATOM	662	OE1	GLŬ	Α	153	67.563	15.977	28.746	1.00	54.51	A
	ATOM	663	OE2	GLU	A	153	65.924	14.500	28.689	1.00	52.47	A
	ATOM	664	C	GLU			66.258	16.455	24.073	1.00	32.91	A
	ATOM	665	0	GLU	А	153	66.304	17.524	23.457	1.00	31.19	Α
5	ATOM	666	N	LYS			66.959	15.376	23.710	1.00	30.19	Α
•	ATOM	667	CA	LYS			67.898	15.431	22.582	1.00	26.56	A
	ATOM	668	CB	LYS			69.323	15.414	23.121	1.00	24.92	A
	ATOM	669	CG	LYS			69.630	16.551	24.041	1.00	23.66	Α
	ATOM	670	CD	LYS			70.944	16.355	24.750	1.00	20.95	Α
10	ATOM	671	CE	LYS			71.274	17.583	25.576	1.00	18.98	Α
10	ATOM	672	NZ	LYS			72.491	17.388	26.360		19.19	
•	ATOM	673	C	LYS			67.806	14.374	21.487		25.00	
	ATOM	674	ō	LYS			67.342	13.257	21.701		25.62	
	ATOM	675	И	LEU			68.276	14.759	20.308		23.36	
15	ATOM	676	CA	LEU			68.337	13.881	19.140	1.00	22.19	A
13	ATOM	677	CB	LEU			67.946	14.624	17.864		21.64	
	ATOM	678	CG	LEU			66.539	15.167	17.707		22.58	
		679		LEU			66.437	15.847	16.350		22.74	
	MOTA	680		LEU			65.533	14.034	17.815		23.23	
20	MOTA	681	CD2	LEU			69.798	13.474	19.004		20.69	
20	ATOM		0	LEU			70.693	14.287	19.249		21.61	
	MOTA	682 683	N	TYR			70.035	12.238	18.592		18.69	
	MOTA ATOM	684	CA	TYR			71.393	11.737	18.431		18.65	
	ATOM	685	CB	TYR			71.690	10.661	19.489		18.51	
25	ATOM	686	CG			156	71.602	11.148	20.913		17.86	
23	ATOM	687		TYR			70.372	11.287	21.550		18.38	
	ATOM	688		TYR			70.286	11.752	22.862		18.95	
	ATOM	689		TYR			72.755	11.488	21.621		19.32	
	MOTA	690	CE2			156	72.690	11.957	22.942	1.00	18.14	Α
30	ATOM	691	CZ			156	71.449	12.086	23.551	1.00	18.56	A
50	ATOM	692	OH			156	71.372	12.547	24.838	1.00	18.33	Α
	ATOM	693	C			156	71.640	11.125	17.059	1.00	18.03	A
	ATOM	694	ō			156	70.903	10.250	16.646	1.00	18.18	Α
	ATOM	695	N			157	72.662	11.568	16.338	1.00	17.19	Α
35	ATOM	696	CA			157	72.937	10.934	15.062	1.00	17.15	Α
	ATOM	69.7	CB			157	72.980	11.951	13.918	1.00	21.54	Α
	ATOM	698	CG	PHE	Α	157	71.663	12.638	13.651	1.00	26.82	Α
	ATOM	699	CD1	PHE	Α	157	70.471	12.165	14.221	1.00	30.87	Α
	ATOM	700	CD2	PHE	Α	157	71.617	13.794	12.869	. 1.00	28.42	Α
40	ATOM	701	CE1	PHE	Α	157	69.249	12.845	14.024	1.00	30.45	Α
	ATOM	702	CE2	PHE	Α	157	70.407	14.483	12.661	1.00	29.44	Α
	ATOM	703	CZ	PHE	A	157	69.224	14.008	13.243		30.41	
	ATOM	704	С	PHE	Α	157	74.286	10.244	15.184		16.38	
	MOTA	705	0	PHE	Α	157	75.256	10.883	15.527		17.91	
45	ATOM	706	N	GLY	Α	158	74.347	8.942	14.919		16.20	
	ATOM	707	CA	GLY	A	158	75.614	8.232	15.009		15.78	
	ATOM	708	С	GLY	Α	158	76.322	8.285	13.671		16.51	
	MOTA	709	0	GLY	Α	158	75.876	7.659	12.710		17.95	
	ATOM	710	N			159	. 77.423	9.028	13.600		14.97	
50	MOTA	711	CA	LEU	A	159	78.143	9.177	12.342		15.17	
	MOTA	712	CB	LEU	Α	159	78.264	10.669	12.012		13.14	
	MOTA	713	CG			159	76.989	11.518	12.133		12.95	
	MOTA	714	CD1	LEU	A	159	77.347	13.002	11.872	1.00		
	ATOM	715	CD2	LEU			75.926	11.020	11.138		11.24	
55	ATOM	716	C			159	79.535	8.540	12.300		15.49	
	MOTA	717	0			159	80.136	8.256	13.333		15.76	
	MOTA	718	N			160	80.051	8.313	11.097		14.32	
	MOTA	719	CA			160	81.389	7.759	10.984		14.68	
	ATOM	720	CB	SER	Α	160	81.699	7.386	9.529	1.00	12.79	, A

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	ATOM	721	OG	SER A		81.395	8.432	8.626	1.00 16.15 A
	MOTA	722	C	SER A		82.365	8.823	11.509	1.00 15.82 A
	ATOM	723	0	SER A		82.152	10.029	11.333	1.00 17.75 A
	ATOM	724	N	TYR A		83.418	8.386	12.184	1.00 16.30 A
5	MOTA	725	CA	TYR A		84.399	9.309	12.740	1.00 17.11 A
	ATOM	726	CB	TYR A	161	84.863	8.785	14.100	1.00 16.09 A
	ATOM	727	CG	TYR A	161	86.020	9.529	14.717	1.00 19.80 A
	MOTA	728	CD1	TYR A	161	86.070	10.933	14.700	1.00 18.64 A
	ATOM	729	CE1	TYR A	161	87.091	11.625	15.345	1.00 19.50 A
10	MOTA	730	CD2	TYR A	161	87.032	8.837	15.394	1.00 20.09 A
	ATOM	731	CE2	TYR A	161	88.057	9.517	16.047	1.00 21.66 A
	ATOM	732	CZ	TYR A	161	88.085	10.918	16.022	1.00 23.52 A
	MOTA	733	OH	TYR A	161	89.111	11.600	16.674	1.00 22.64 A
	ATOM	734	C.	TYR A	161	85.594	9.495	11.815	1.00 17.86 A
15	ATOM	735	o	TYR A		86.269	8.527	11.459	1.00 19.30 A
	ATOM	736	N	ALA A		85.854	10.736	11.418	1.00 18.22 A
	ATOM	737	CA	ALA A		86.990	11.040	10.546	1.00 19.59 A
	ATOM	738	CB	ALA A		86.569	12.063	9.466	1.00 19.99 A
	ATOM	739	C	ALA A		88.051	11.629	11.472	1.00 19.11 A
20	ATOM	740	ō	ALA A		88.050	12.828	11.736	1.00 18.81 A
20	ATOM	741	N	ALA A		88.952	10.775	11.956	1.00 18.78 A
	ATOM	742	CA.	ALA A	•	89.994	11.165	12.918	1.00 18.84 A
		743	CB	ALA A		90.867	9.924	13.279	1.00 10.04 A
	ATOM		CP					12.604	1.00 19.04 A
25	ATOM	744		ALA A		90.908	12.357		1.00 16.22 A 1.00 16.79 A
25	ATOM	745	0	ALA A		91.290	13.101	13.508	
	MOTA	746	N	ASN A		91.251	12.560	11.340	1.00 17.46 A
	ATOM	747	CA	ASN A		92.148	13.645	11.023	1.00 17.79 A
	ATOM	748	CB	ASN A		92.990	13.270	9.803	1.00 20.45 A
	ATOM	749	CG	ASN A		93.919	12.092	10.097	1.00 21.08 A
30	ATOM	750		ASN A		94.663	12.117	11.066	1.00 21.57 A
	ATOM	751		ASN A		93.862		9.271	.1.00 24.54 A
	ATOM	752	C	ASN A		91.555	15.044	10.889	1.00 18.34 A
	ATOM	753	0	ASN A		92.293	16.005	10.634	1.00 19.83 A
	ATOM	754	N	GLY A		90.247	15.176	11.083	1.00 15.01 A
35	MOTA	755	CA	GLY A		89.644	16.490	11.022	1.00 15.54 A
	ATOM	756	С	GLY A		89.580	17.212	9.683	1.00 17.67 A
	ATOM	757	0	GLY A	165	89.607	16.600	8.613	1.00 19.49 A
	MOTA	758	N	GLU A		89.510	18.534	9.753	1.00 17.46 A
	ATOM	759	CA	GLU A		89.378	19.379	8.577	1.00 19.26 A
40	ATOM	760	CB	GLU A		89.064	20.805	9.019	1.00 21.87 A
•	ATOM	761	CG	GLU A	166	88.057	20.917	10.149	1.00 24.70 A
	MOTA	762	CD	GLU A		87.723	22.359	10.477	1.00 26.05 A
•	MOTA	763	OE1	GLU A	166	88.469	23.251	10.001	1.00 25.93 A
	MOTA	764	OE2	GLU A	166	86.726	22.598	11.213	1.00 25.24 A
45	ATOM	765	C	GLU A	166	90.538	19.441	7.592	1.00 20.11 A
	ATOM	766	0	GLU A	166	91.707	19.501	7.978	1.00 22.88 A
	ATOM	767	N	LEU A	167	90.195	19.443	6.312	1.00 18.72 A
	ATOM	768	CA	LEU A	167	91.173	19.565	5.242	1.00 17.38 A
	ATOM	769	CB	LEU A	167	90.463	19.516	3.888	1.00 15.71 A
50	ATOM	770	CG	LEU A		91.238	19.817	2.601	1.00 15.42 A
	MOTA	771	CD1	LEU A	167	92.242	18.704	2.343	1.00 14.98 A
	MOTA	772		LEU A		90.265	19.947	1.416	1.00 12.32 A
	ATOM	773	C.	LEU A		91:817	20.940	5.438	1.00 19.75 A
	ATOM	774	0	LEU A		93.030	21.103	5.266	1.00 19.61 A
55	ATOM	775	N	LEU A		91.001	21.928	5.812	1.00 20.53 A
	ATOM	776	CA	LEU A		91.516	23.277	6.033	1.00 22.20 A
	ATOM	777	CB	LEU A		90.436	24.192	6.637	1.00 20.41 A
	ATOM	778	CG	LEU A		90.923	25.611	7.024	1.00 21.71 A
	ATOM	779		LEU A		91.275	26.413	5.768	1.00 20.09 A
	ATOM		CDI	א טריד	. 100	12.213	20.473		

	MOTA	780	CD2	LEU 2	A 168	89.837	26.341	7.797	1.00 20.84 A
	ATOM	781	С	LEU 2	A 168	92.731	23.245	6.968	1.00 23.07 A
	MOTA	782	0	LEU 2	A 168	93.636	24.054	6.838	1.00 22.18 A
	ATOM	783	N	LYS 2	A 169	92.742	22.305	7.905	1.00 24.67 A
5	MOTA	784	CA	LYS 2	A 169	93.844	22.192	8.850	1.00 28.56 A
	MOTA	785	CB.		A 169	93.561	21.076	9.858	1.00 31.12 A
	MOTA	786	CG	LYS 2	A 169	94.615	20.933	10.938	1.00 35.60 A
	MOTA	787	CD	LYS .	A 169	94.436	19.652	11.765	1.00 39.37 A
	MOTA	788	CE		A 169	94.832	18.410	10.961	1.00 42.26 A
10	ATOM	789	NZ	LYS .	A 169	94.664	17.131	11.725	1.00 42.83 A
	MOTA	790	С	LYS .	A 169	95.151	21.902	8.119	1.00 29.24 A
	ATOM	791	0	LYS .	A 169	96.190	22.505	8.398	1.00 30,32 A
	MOTA	792	N	TYR .	A 170	95.101	20.970	7.179	1.00 29.12 A
	ATOM	793	CA	TYR .	A 170	96.290	20.619	6.423	1.00 28.18 A
15	ATOM	794	CB	TYR .	A 170	96.037	19.344	5.637	1.00 25.30 A
	ATOM	795	CG	TYR .	A 170	95.926	18.182	6.569	1.00 27.01 A
	ATOM	796	CD1	TYR	A 170	97.072	17.533	7.053	1.00 26.92 A
	ATOM	797	CE1	TYR	A 170	96.974	16.532	8.008	1.00 25.37 A
	MOTA	798	CD2	TYR.	A 170	94.688	17.792	7.062	1.00 25.14 A
20	ATOM	799	CE2	TYR	A 170	94.580	16.807	8.009	1.00 26.49 A
	ATOM	800	CZ	TYR	A 170	95.720	16.179	8.484	1.00 26.98 A
	MOTA	801	OH	TYR	A 170	95.580	15.223	9.456	1.00 27.66 A
	ATOM	802	C	TYR	A 170	96.690	21.742	5.507	1.00 28.69 A
	ATOM	803	0	TYR	A 170	97.875	21.971	5.285	1.00 30.98 A
25	MOTA	804	N	ILE	A 171	95.705	22.452	4.976	1.00 28.95 A
•	ATOM	805	CA	ILE	A 171	96.006	23.550	4.088	1.00 29.79 A
	ATOM	806	CB	ILE	A 171	94.721	24.233	3.579	
	MOTA	807	CG2	ILE	A 171	95.082	25.439	2.714	1.00 28.21 A
	ATOM	808			A 171	93.906	23.227	2.747	1.00 29.66 A
30	MOTA	809	CD1	ILE	A 171	92.567	23.754	2.224	1.00 29.13 A
	MOTA	810	С	ILE	A 171	96.897	24.536	4.833	1.00 31.13 A
	MOTA	811	0		A 171	97.925	24.956	4.300	1.00 30.93 A
	MOTA	812	И		A 172	96.525	24.862	6.075	1.00 32.00 A
	MOTA	813	CA		A 172	97.294	25.789	6.903	1.00 32.60 A
35	MOTA	814	CB		A 172	96.527	26.175	8.163	1.00 32.77 A
	MOTA	815	CG		A 172	95.257	26.982	7.972	1.00 38.24 A
	MOTA	816	CD		A 172	94.853	27.602	9.335	1.00 43 47 A
	ATOM	817	NE		A 172	93.501	28.181	9.412	1.00 46.65 A
	MOTA	818	CZ.		A 172	92.903	28.888	8.448	1.00 47.62 A
40	MOTA	819			A 172	93.517	29.115	7.287	1.00 47.16 A
	ATOM	820			A 172	91.691	29.398	8.659	1.00 45.61 A
	ATOM	821	С		A 172	98.646	25.219	7.338	1.00 32.95 A 1.00 34.27 A
	ATOM	822	0		A 172	99.644	25.920	7.311	1.00 34.27 A
	ATOM	823	N		A 173	98.674	23.960	7.761	
45	ATOM	824	CA		A 173	99.912	23.341	8.209	
	MOTA	825	CB		A 173	99.668	21.896	8.619	1.00 32.72 A 1.00 33.67 A
	MOTA	826	C.		A 173	101.005	23.400	7.152	
,	MOTA .	827	0		A 173	102.125	23.817	7.438	1.00 33.78 A 1.00 33.50 A
.	MOTA	828	N	_	A 174	100.698	22.995	5.926 4.896	1.00 33.50 A 1.00 33.22 A
50	MOTA	829	CA		A 174	101.728	23.030		1.00 33.22 A 1.00 33.98 A
	MOTA	. 830	CB		A 174	101.731	21.736	4.043 4.950	1.00 33.98 A 1.00 32.94 A
	MOTA	831	CG2		A 174	101.725	20.502		1.00 32.94 A 1.00 33.93 A
	ATOM	832			A 174	100.517	21.709	3.125 2.080	1.00 35.93 A 1.00 36.79 A
 -	ATOM	833	_		A 174	100.602	20.631	3.957	1.00 36.79 A 1.00 32.69 A
55	MOTA	. 834	C		A 174	101.638	24.231 24.269	2.938	1.00 32.05 A
	MOTA	835	0		A 174	102.326	25.204	4.287	1.00 33.00 A
	MOTA	836	N		A 175		26.386	3.446	1.00 31.70 A
	MOTA	837	CA		A 175		26.388	2.184	1.00 32.03 A
	МОТА	838	С	ZLI D	A 175	22.030	20.223	0 -3	

	ATOM	839	0	GLY A	A 175	98.870	26.958	1.976	1.00 35.12 A
	MOTA	840	N	SER A	A 176	100.225	25.291	1.322	1.00 31.63 A
	MOTA	841	CA	SER Z	A 176	99.489	25.018	0.091	1.00 31.11 A
	ATOM	842	CB	SER A	A 176	99.810	26.040	-0.996	1.00 31.54 A
5	ATOM	843	OG	SER I	A 176	101.141	25.874	-1.464	1.00 33.96 A
	ATOM	844	C	SER Z	A 176	99.946	23.640	-0.354	1.00 30.72 A
	ATOM	845	0	SER A	A 176	100.977	23.154	0.111	1.00 31.29 A
	ATOM	846	N	PHE A	A 177	99.180	23.018	-1.246	1.00 28.27 A
	ATOM	847	CA	PHE .	A 177	99.475	21.683	-1.738	1.00 26.97 A
10	ATOM	848	CB	PHE	A 177	98.169	20.948	-2.060	1.00 27.18 A
	ATOM	849	CG	PHE .	A 177	97.376	20.530	-0.854	1.00 27.90 A
	ATOM	850	CD1	PHE .	A 177	97.551	21.155	0.379	1.00 26.91 A
	ATOM	851	CD2	PHE .	A 177	96.432	19.503	-0.957	1.00 27.62 A
	ATOM	852			A 177	96.812	20.762	1.477	1.00 26.03 A
15	ATOM	853			A 177	95.684	19.106	0.144	1.00 23.95 A
	ATOM	854	CZ		A 177	95.873	19.730	1.357	1.00 25.81 A
	ATOM	855	C		A 177	100.299	21.726	-3.008	1.00 26.99 A
	ATOM	856	ō		A 177	100.115	22.618	-3.832	1.00 27.45 A
	ATOM	857	N		A 178	101.200	20.762	-3.179	1.00 26.09 A
20	ATOM	858	CA		A 178	101.967	20.704	-4.411	1.00 26.09 A
20	ATOM	859	CB		A 178	103.135	19.730	-4.303	1.00 27.73 A
	ATOM	860	CG		A 178	102.689	18.318	-4.023	1.00 33.79 A
	ATOM	861			A 178	101.601	17.919	-4.510	1.00 37.57 A
	ATOM	862			A 178	103.431	17.590	-3.324	1.00 35.89 A
25	ATOM	863	C		A 178	100.955	20.202	-5.443	1.00 25.72 A
23	ATOM	864	Ö		A 178	99.763	20.063	-5.128	1.00 24.80 A
	ATOM	865	N		A 179	101.419	19.897	-6.650	1.00 24.80 A
	ATOM	866	CA		A 179	100.514	19.444	-7.697	1:00 25.67 A
	ATOM	867	CB		A 179	101.187	19.554	-9.052	1.00 27.44 A
30	ATOM	868	CG		A 179	100.197	19.921	-10.129	1.00 31.17 A
50	ATOM	869	CD		A 179	100.823	19.999	-11.492	1.00 35.24 A
	ATOM	870			A 179	102.016		-11.572	1.00 35.82 A
	ATOM	871			A 179	100.116	19.707	-12.488	1.00 38.12 A
	ATOM	872	C		A 179	99.917	18.041	-7.560	1.00 24.90 A
35	ATOM	873	ō		A 179	98.755	17.822	-7.894	1.00 23.01 A
33 ,	ATOM	874	N		A 180	100.709	17.095	-7.082	1.00 24.57 A
	ATOM	875	CA		A 180	100.240	15.723	-6.923	1.00 25.53 A
	ATOM	876	СВ		A 180	101.395	14.803	-6.478	1.00 24.65 A
	ATOM	877			A 180	102.525	15.069	-7.304	1.00 25.84 A
40	ATOM	878			A 180	101.021	13.334	-6.624	1.00 23.39 A
40	ATOM	879	c		A 180	99.110	15.623	-5.902	1.00 25.85 A
	ATOM	880	Ö		A 180	98.149	14.892	-6.111	1.00 25.59 A
	ATOM	881	N		A 181	99.237	16.359	-4.799	1.00 25.83 A
	ATOM	882	CA		A 181	98.217	16.355	-3.752	1.00 26.26 A.
45	ATOM	883	СВ		A 181	98.778	16.939	-2.451	1.00 27.81 A
43	ATOM	884	SG		A 181	100.202	16.031		1.00 32.72 A
	ATOM	885			A 181	96.963	17.127		1.00 25.20 A
	ATOM	886	ō		A 181	95.853	16.696		1.00 26.19 A
	ATOM	887	Ŋ		A 182	97.139	18.262	-4.841	1.00 22.74 A
50	ATOM	888	CA		A 182	96.002	19.046		1.00 21.82 A
50	ATOM	889	CB		A 182	96.453	20.308		1.00 21.81 A
	ATOM	890			A 182	97.258	21.161		1.00 24.55 A
	MOTA	891	CG2		A 182	95.252	21.080		1.00 18.62 A
	ATOM	892	C		A 182	95.197	18.141		1.00 23.45 A
55	ATOM	893	Ö		A 182	93.975	17.997		1.00 22.94 A
	ATOM	894	N		A 183	95.897	17.528		1.00 22.71 A
	ATOM	895	CA		A 183	95.260	16.648		1.00 23.26 A
	ATOM	896	CB		A 183	96.285	16.118		1.00 22.46 A
	ATOM	897	CG		A/183	95.692		-10.184	1.00 24.96 A
	23.4.01.1	001				•	-,-		

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	ATOM	898	CD	ARG	A	183	96.762	14.512		1.00 27.09 A
	ATOM	899	NE	ARG	A	183	97.372	15.577	-11.849	1.00 33.02 A
	ATOM	900	CZ	ARG	A	183	98.637	15.948		1.00 33.62 A
	ATOM	901	NHl	ARG			99.440	15.312		1.00 32.57 A
5	MOTA	902	NH2	ARG			99.069	17.006		1.00 33.25 A
	ATOM	903	C	ARG			94.559	15.475	-7.459	1.00 22.42 A
•	MOTA	904	0	ARG			93.393	15.193	-7.721	1.00 21.37 A
	MOTA	905	N	PHE			95.255	14.800	-6.562	1.00 21.19 A
	MOTA	906	CA	PHE			94.630	13.673	-5.888	1.00 22.20 A
10	MOTA	907	CB	PHE			95.615	12.964	-4.966	1.00 23.58 A
	MOTA	908	CG	PHE			95.029	11.766	-4.283	1.00 25.43 A
	ATOM	909		PHE			94.916	10.556	-4.954	1.00 25.01 A
	ATOM	910		PHE			94.508	11.867	-2.998	1.00 24.35 A
	ATOM	911		PHE			94.285	9.460	-4.356	1.00 23.50 A
15	ATOM	912		PHE			93.881	10.782	-2.409	1.00 24.71 A
	ATOM	913	CZ	PHE			93.771	9.577	-3.094	1.00 22.95 A
	ATOM	914	C	PHE			93.405	14.074	-5.072	1.00 21.96 A
	ATOM	915	0	PHE			92.348	13.450	-5.170	1.00 21.31 A
	ATOM	916	N	TYR			93.544	15.116	-4.267	1.00 21.18 A
20	ATOM	917	CA	TYR			92.433	15.543	-3.445	1.00 20.50 A
	ATOM	918	CB	TYR			92.956	16.425		1.00 21.33 A
	ATOM	919	CG	TYR			93.494	15.550	-1.190	1.00 22.24 A
	ATOM	920				185	92.641	14.670	-0.507	1.00 21.55 A
~-	ATOM	921		TYR			93.127	13.755	0.414	1.00 20.71 A
25	ATOM	922	CD2	TYR			94.853	15.497	-0.904	1.00 21.37 A 1.00 21.80 A
	ATOM	923	CE2	TYR			95.353 94.486	14.579	0.019 0.670	1.00 21.80 A
	ATOM	924	CZ	TYR				13.705 12.746	1.519	1.00 21.18 A
	ATOM	925	G ·	TYR TYR			94.986 91.273	16.182	-4.201	1.00 19.04 A
30	ATOM	926	0	TYR			90.112	16.162	-3.801	1.00 13.27 A
30	ATOM	927 928	Ŋ	THR			91.576	16.834	-5.314	1.00 17.72 A 1.00 17.25 A
	ATOM	928	CA	THR			90.527	17.433	-6.110	1.00 17.23 A
	ATOM	930	CB	THR			91.097	18.366	-7.188	1.00 15.69 A
	ATOM ATOM	931		THR			91.710	19.508	-6.564	1.00 16.11 A
35	ATOM	932	CG2	THR			89.996	18.816	-8.135	1.00 12.68 A
33	ATOM	933	C	THR		•	89.756	16.302	-6.785	1.00 15.75 A
	ATOM	934	0	THR			88.523	16.350	-6.899	1.00 16.51 A
	ATOM	935	Ŋ	ALA			90.478	15.277	-7.218	1.00 14.94 A
	ATOM	936	CA	ALA			89.841	14.136	-7.868	1.00 16.15 A
40	ATOM	937	CB	ALA			90.905	13.130	-8.382	1.00 13.30 A
	ATOM	938	C	ALA			88.847	13.450	-6.911	1.00 16.71 A
	ATOM	939	o	ALA			87.743	13.075	-7.328	1.00 16.50 A
	ATOM	940	N	GLU			89.213	13.308	-5.635	1.00 17.10 A
	ATOM	941	CA	GLU			88.302	12.673	-4.679	1.00 17.85 A
45	ATOM	942	CB	GLU	Α	188	88.953	12.514	-3.302	1.00 18.83 A
•	ATOM	943	CG	GLU			90.219	11.665	-3.296	1.00 19.46 A
	ATOM	944	CD	GLU	·A	188	90.370	10.795	-2.050	1.00 20.84 A
	ATOM	945	OE1	GLU		*	90.131	11.276	-0.920	1.00 21.14 A
	ATOM	946	OE2	GLU	A	188	90.749	9.616	-2.207	1.00 23.35 A
50	ATOM	947	С	GLU	Α	188	87.043	13.516	-4.551	1.00 17.79 A
	ATOM	948	0	GLU	Α	188	85.921	13.005	-4.579	1.00 18.83 A
	ATOM	949	N	ILE	A	189	87.220	14.824	-4.449	1.00 17.09 A
	MOTA	950	CA	ILE	Α	189	86.060	15.688	-4.312	1.00 15.61 A
	ATOM	951	CB	ILE	A	189	86.495	17.141	-4.054	1.00 15.83 A
55	MOTA	952	CG2	ILE	A	189	85.278	18.019	-3.853	1.00 14.16 A
	MOTA	953		ILE			87.380	17.199	-2.794	1.00 17.34 A
	MOTA	954	CD1	ILE			87.949	18.583	-2.479	1.00 15.37 A
	ATOM	955	C			189	85.176	15.611	-5.558	1.00 16.00 A
	ATOM	956	0	ILE	Α	189	83.953	15.530	-5.460	1.00 15.52 A

	ATOM	957	N	VAL	A 190	85.794	15.619	-6.733	1.00	15.46	А
	MOTA	958	CA		A 190					15.38	
	ATOM	959	CB		A 190					15.37	
	ATOM	960	CG		A 190			-10.447		14.43	
5	ATOM	-961			A 190					14.03	
	ATOM	962			A 190						
	ATOM	963			A 190					17.35	
	ATOM	964			A 191			-8.258		15.96	
	ATOM	965						-7.683		17.90	
10	ATOM				A 191			-7.660		17.77	
10		966			A 191			-7.344		18.25	
	ATOM	967			A 191	84.801	9.523	-7.243		21.13	
	ATOM	968			A 191	83.147	11.778	-6.640	1.00	17.28	Α
	ATOM	969			A 191	82.153	11.095	~6.865	1.00	15.44	A
	MOTA	970	И		A 192	83.291	12.490	-5.525		17.27	
15	ATOM	971	· CA	ALA A	A 192	82.267	12.529	-4.485		15.98	
	MOTA	972	CB	ALA A	A 192	82.834		-3.191		14.89	
	MOTA	973	C	ALA A	A 192	81.078		-4.988		16.44	
	ATOM	974	0	ALA A		79.934	12.922	-4.816		17.59	
	ATOM	975	N	LEU A		81.340	14.487	-5.609		16.63	
20	ATOM	976	CA	LEU A		80.253	15.303	-6.140		16.11	
	ATOM	977	СВ	LEU A		80.769					
	ATOM	978	CG	LEU A			16.632	-6.688		16.40	
	ATOM	979	CD:			81.421	17.545	-5.645		18.83	
	ATOM	980		LEU A		81.779	18.885	-6.276		18.24	
25	ATOM	981	C			80.455	17.751	-4.479	1.00	18.63	A
23 .	ATOM			LEU A		79.509	14.551	-7.236	1.00	16.95	Α
	ATOM	982	0	LEU A		78.286	14.623	-7.325	1.00	18.76	Α
	ATOM	983	N	GLU A		80.229	13.825	-8.079		17.87	
		984	CA	GLU A	194	79.539	13.082	-9.124	1.00	19.66	Α
30 -	ATOM	985	CB			80.525	12.295	-9.990	1.00	21.82	Α
30 ~	ATOM	986	CG	GLU A		79.844	11.333	-10.947	1.00	21.12	Α
	MOTA	987		GLU A	194	80.831	10.513	-11.758		25.70	
	MOTA	988	OE1	GLU A	194	81.900	10.122	-11.216		27.41	
	ATOM	989		GLU A	194	80.527		-12.939		26.12	
	MOTA	990	С	GLU A		78.546	12.123	-8.479		19.58	
35	MOTA	991	0	GLU A	194	77.420	11.987	-8.937		17.78	
	ATOM	992	N	TYR A	195	78.962	11.462	-7.406		19.09	
	MOTA	993	CA	TYR A	195	78.063	10.545	-6.736		19.86	
	ATOM	994	CB	TYR A		78.807	9.740	-5.673		20.01	
	MOTA	995	CG	TYR A		77.871	8.975	-4.756		20.01	
40	ATOM	996	CD1	TYR A		77.329	7.748	-5.142			
	ATOM	997		TYR A		76.471	7.044			19.40	
	ATOM	998	CD2			77.527		-4.296		18.43	
	ATOM	999	CE2			76.678	9:482	-3.500		20.11	
	ATOM	1000	CZ	TYR A		76.154	8.792	-2.652		19.96	
45	ATOM	1001		TYR A		75.336	7.567	-3.057		21.07	
	ATOM	1002	C				6.859	-2.206		21.31	
	ATOM	1003	ō	TYR A		76.914	11.295	-6.060		20.00	
	ATOM	1003		TYR A		75.775	10.823	-6.033	1.00 2	21.42	A
			N	LEU A		77.222	12.455	-5.500	1.00	17.38	A
50	ATOM	1005	CA	LEU A		76.209	13.226	-4.795	1.00	18.74	A
50	ATOM	1006	CB	LEU A		76.846	14.412	~4.049	1.00	17.38 2	A.
	ATOM	1007	CG	LEU A	196	75.850	15.100	-3.110		19.04 2	
	ATOM	1008	CD1	LEU A	196	75.423	14.093	-2.061		17.66	
•	ATOM	1009		LEU A	196	76.462	16.338	-2.453		19.54 7	
	MOTA	1010	C	LEU A		75.148	13.747	-5.751		18.47 2	
55 ·	MOTA	1011	0	LEU A	196	73.944	13.608	-5.523		15.05 A	
	MOTA	1012	N	HIS A		75.622	14.361	-6.824		18.35	
	ATOM	1013	CA	HIS A	197	74.740	14.915	-7.812		20.04 7	
	MOTA	1014	CB	HIS A		75.562	15.809	-8.718		20.29	
7	MOTA	1015	CG	HIS A		76.048	17.044	-8.025		21.90 F	
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	ATOM	1016	CD2	HIS A	197		75.766	17.539	-6.794	1.00 19.49 A
	ATOM	1017	ND1	HIS A	197		76.892	17.956	-8.621	1.00 20.69 A
	MOTA	1018	CE1	HIS A	197		77.104	18.960	-7.789	1.00 20.86 A
	ATOM	1019	NE2	HIS A	197		76.433	18.732	-6.676	1.00 19.12 A
5	ATOM	1020	С	HIS A	197		73.950	13.858	-8.587	1.00 21.27 A
-	ATOM	1021	0	HIS A			72.865	14.133	-9.099	1.00 21.23 A
	ATOM	1022	N	GLY A			74.487	12.644	-8.644	1.00 21.36 A
	ATOM	1023	CA	GLY A		. •	73.810	11.569	-9.339	1.00 20.60 A
	ATOM	1024	C	GLY A			72.528	11.203	-8.632	1.00 22.72 A
10	ATOM	1025	Ō	GLY A			71.593	10.742	-9.269	1.00 22.75 A
	MOTA	1026	N	LYS A			72.478	11.411	-7.313	1.00 24.27 A
	ATOM	1027	CA	LYS A			71.280	11.105	-6.523	1.00 22.95 A
	ATOM	1028	CB	LYS A			71.659	10.629	-5.123	1.00 24.67 A
	ATOM	1029	CG	LYS A			72.570	9.429	-5.109	1.00 29.22 A
15	ATOM	1030	CD	LYS A			72.986	9.064	-3.701	1.00 33.11 A
13	ATOM	1031	CE	LYS A			72.531	7.660		1.00 37.28 A
	ATOM	1032	NZ	LYS A			72.917	6.686	-4.455	1.00 38.82 A
	ATOM	1032	C	LYS A			70.432	12.354	-6.398	1.00 22.39 A
	ATOM	1033	Ö	LYS A			69.558	12.431	-5.542	1.00 22.53 A
20	ATOM	1035	И	GLY A			70.710	13.343	-7.241	1.00 21.56 A
20	ATOM	1035	CA	GLY A		•	69.953	14.580	-7.203	1.00 22.28 A
	ATOM	1037	C	GLY A			70.006	15.326	-5.882	1.00 23.53 A
	ATOM	1037	0	GLY A			69.017	15.930	-5.461	1.00 24.83 A
		1039	И	ILE A			71.161	15.302	-5.225	1.00 22.74 A
25	ATOM	1039	CA	ILE A			71.314	15.985	-3.951	1.00 22.95 A
23	ATOM	1040	CB	ILE A			71.796	15.007	-2.842	1.00 22.51 A
	MOTA MOTA	1041	CG2	ILE A			71.795	15.757	-1.536	1.00 21.73 A
				ILE A			70.788	13.876	-2.638	1.00 22.48 A
	MOTA	1043		ILE A			71.274	12.791	-1.687	1.00 17.26 A
20	ATOM		CDI	ILE A			72.361	17.086	-4.076	1.00 24.41 A
30	MOTA	1045					73.387	16.904	-4.737	1.00 26.41 A
	MOTA	1046	0	ILE A			72.118	18.236	-3.470	1.00 23.00 A
	MOTA	1047	N				73.137	19.267	-3.520	1.00 24.60 A
	MOTA	1048	CA	ILE A			72.729	20.440	-4.420	1.00 26.37 A
25	MOTA	1049	CB	ILE A			72.723	19.934	-5.829	1.00 28.52 A
35	ATOM	1050	CG2	ILE A			72.303	21.086	-3.922	1.00 29.04 A
	MOTA	1051	CG1	ILE A			70.958	22.165	-4.845	1.00 23.01 A
	MOTA	1052		ILE A				19.732	-2.105	1.00 32.35 A
	ATOM	1053	C	ILE A			73.482	19.732	-1.257	1.00 25.89 A
40	ATOM	1054		ILE A			72.605 74.776	19.882	-1.856	1.00 23.03 A 1.00 22.94 A
40	ATOM	1055		HIS A				20.273	-0.555	1.00 22.27 A
	ATOM	1056	CA	HIS A			75.289		-0.526	1.00 22.27 A 1.00 20.00 A
	ATOM	1057	CB	HIS A			76.800	20.010 20.051	0.840	1.00 20.00 A 1.00 18.45 A
	ATOM	1058	CG	HIS A			77.401		1.640	1.00 10.43 A 1.00 19.77 A
٠	MOTA	1059		HIS A			77.865	19.060		1.00 15.77 A 1.00 16.33 A
45	ATOM	1060		HIS A			77.569	21.222	1.542	1.00 18.33 A 1.00 17.77 A
	ATOM	1061		HIS A			78.115	20.953	2.715	1.00 17.77 A
	MOTA	1062		HIS A			78.306	19.650	2.800	
:	MOTA	1063	C	HIS P			74.978	21.731	-0.206	1.00 23.37 A
	MOTA	1064	0	HIS F		•	74.411	22.009	0.860	1.00 22.52 A
50	MOTA	1065	N	ARG A			75.361	22.648	-1.101	1.00 23.22 A
	MOTA	1066	CA	ARG A			75.126	24.087	-0.934	1.00 23.42 A
	MOTA	1067	CB	ARG A			73.674	24.375	-0.544	1.00 22.74 A
	ATOM	1068	CG	ARG A			72.663		-1.561	1.00 24.57 A
	MOTA	1069	CD	ARG A			71.341	24.681	-1.325	1.00 26.51 A
55	MOTA	1070	NE	ARG A			70.699	24.299	-0.074	1.00 28.25 A
	MOTA	1071	CZ	ARG A			69.596	24.871	0.405	1.00 28.63 A
	MOTA	1072		ARG A			69.013	25.849	-0.267	1.00 28.47 A
	MOTA	1073		ARG A			69.086	24.472	1.563	1.00 28.55 A
	MOTA	1074	C	ARG A	204		76.017	24.819	0.061	1.00 24.12 A

	MOTA	1075	0	ARG 2	A :	204	75.805	26.001	0.308	1.00 26.26 A
	MOTA	1076	N	ASP 3	A :	205	76.990	24.135	0.654	1.00 23.05 A
	ATOM	1077	CA	ASP :	A :	205 -	77.887	24.789	1.595	1.00 20.96 A
	MOTA	1078	CB	ASP .	A :	205	77.219	24.883	2.964	1.00 22.31 A
5	MOTA	1079	CG	ASP .	A :	205	77.964	25.801	3.914	1.00 26.08 A
_	ATOM	1080	OD1	ASP .	A :	205	78.812	26.582	3.439	1.00 25.93 A
	ATOM	1081	OD2	ASP .	A :	205	77.707	25.751	5.141	1.00 29.89 A
	MOTA	1082	C	ASP .			79.210	24.020	1.662	1.00 20.46 A
	ATOM	1083	Ō	ASP .			79.812	23.833	2.716	1.00 21.36 A
10	ATOM	1084	И	LEU .			79.666	23.584	0.504	1.00 18.98 A
	ATOM	1085	CA	LEU .	A :	206	80.893	22.827	0.407	1.00 19.83 A
	MOTA	1086	CB	LEU .			80.983	22.229	-0.994	1.00 21.73 A
	ATOM	1087	CG	LEU			82.039	21.167	-1.298	1.00 24.76 A
	ATOM	1088		LEU			81.818	19.943	-0.401	1.00 24.95 A
15	ATOM	1089		LEU.			81.941	20.789	-2.778	1.00 23.74 A
	ATOM	1090	C	LEU			82.093		0.691	1.00 20.17 A
	ATOM	1091	ō	LEU			82.162		0.200	1.00 20.92 A
	ATOM	1092	Ŋ	LYS			83.044		1.475	1.00 19.79 A
	ATOM	1093	CA	LYS			84.233		1.821	1.00 19.45 A
20	ATOM	1094	CB	LYS			83.825		2.667	1.00 17.84 A
20	ATOM	1095	CG	LYS			83.123		3.933	1.00 19.19 A
	ATOM	1096	CD	LYS			82.331		4.500	1.00 20.50 A
	ATOM	1097	CE	LYS			81.663		5.797	1.00 22.10 A
	MOTA	1098	NZ	LYS			80.955		6.480	1.00 22.34 A
25	ATOM	1099	C	LYS			85.241		2.565	1.00 19.59 A
23	MOTA	1100	ο.	LYS			84.917		2.985	1.00 20.21 A
	ATOM	1101	Ŋ	PRO			86.480		2.737	1.00 19.79 A
	ATOM	1101	CD	PRO			87.032		2.188	1.00 18.04 A
	MOTA	1102	CA	PRO			87.526		3.428	1.00 19.22 A
30	ATOM	1103	CB	PRO			88.75		3.297	1.00 19.27 A
30		1104	CG	PRO			88.496	•	2.027	
	MOTA	1105	Ċ	PRO			87.22		4.883	1.00 20.50 A
	ATOM ATOM	1100	0	PRO			87.79		5.411	1.00 21.44 A
	ATOM	1107	И	GLU			86.33		5.530	1.00 20.19 A
35	ATOM	1109	CA	GLU			85.95		6.927	
33		1110	CB	GLU			85.383			1.00 21.43 A
	ATOM	1111	CG	GLU			86.33		7.535	1.00 26.33 A
	ATOM	1112	CD	GLU			86.20		6.270	1.00 30.17 A
	MOTA			GLU			86.14		5.131	1.00 30.44 A
40	ATOM	1113 1114		GLU			86.17		6.422	1.00 33.49 A
40	MOTA			GLU			84.92		7.040	1.00 22.45 A
	MOTA	1115	C	GLU			84.73		8.114	1.00 21.98 A
	MOTA	1116	0	ASN			84.26			1.00 22.73 A
	ATOM	1117	N	ASN			83.23		5.788	1.00 23.66 A
45	ATOM	1118	CA				82.10			
45	ATOM	1119	CB	ASN			81.10		5.613	1.00 33.39 A
	ATOM	1120	CG	ASN			80.22			1.00 36.52 A
	ATOM	1121		ASN					_	1.00 34.23 A
	ATOM	1122		ASN			81.22 83.77			1.00 31.23 H
	MOTA	1123	C	ASN			83.06			1.00 21.16 A
50	ATOM	1124		ASN						1.00 19.42 A
	MOTA	1125	N			211	85.00 85.00			1.00 13.42 A
	MOTA	1126	CA			211	85.61		•	1.00 17.45 A
	ATOM	1127	CB			211	86.31 87.04			1.00 12.68 A
	ATOM	1128		ILE			87.04 85.27			1.00 12.00 A
55	MOTA	1129		ILE						1.00 10.47 A
	MOTA	1130		ILE			85.85 86.62			1.00 10.47 A
	ATOM	1131	C			211				1.00 17.05 A
	MOTA	1132	0			211	87.68			1.00 17.70 A
	MOTA	1133	N	LEU	Ą	212	86.26	5 16.457	5.033	2.00 10.00 A

	7.0014	7774	G 3			272		07 101	3E 073	C CEC	1.00 15.84 A
•	ATOM	1134	CA	LEU				87.121	15.871	6.656	
	ATOM	1135	CB	LEU				86.256	15.319	7.793	1.00 14.28 A
	MOTA	1136	CG	LEU	Α	212		85.108	16.227	8.285	1.00 14.68 A
	ATOM	1137		LEU				84.606	15.715	9.647	1.00 11.38 A
5	MOTA	1138	CD2	LEU	Α	212		85.579	17.685	8.422	1.00 10.88 A
	MOTA	1139	С	LEU	Α	212		88.031	14.787	6.114	1.00 16.77 A
	MOTA	1140	0	LEU	A	212		87.861	14.335	4.984	1.00 16.78 A
	ATOM	1141	N	LEU	Α	213		88.999	14.374	6.925	1.00 16.47 A
	MOTA	1142	CA	LEU	Α	213		89.924	13.332	6.516	1.00 17.64 A
10	ATOM	1143	CB	TEU	Α	213		91.323	13.926	6.378	1.00 18.08 A
	ATOM	1144	CG	LEU				91.367	14.880	5.176	1.00 17.92 A
	ATOM	1145		LEU				92.076	16.134	5.529	1.00 18.78 A
	ATOM	1146		LEU				92.042	14.187	4.000	1.00 17.07 A
	ATOM	1147	C	LEU				89.919	12.147	7.473	1.00 18.68 A
15	ATOM	1148	ō	LEU				90.091	12.297	8.672	1.00 18.75 A
15	ATOM	1149	N	ASN				89.712	10.955	6.939	1.00 21.19 A
	ATOM	1150	CA	ASN				89.673	9.780	7.797	1.00 23.68 A
			CB	ASN				88.864	8.657	7.122	1.00 25.68 A
	ATOM	1151	CG	ASN				89.613	7.979	6.012	1.00 23.00 H
20	MOTA	1152						90.680	8.426	5.590	1.00 31.70 A
20	ATOM	1153		ASN						5.521	1.00 35.54 A
	ATOM	1154		ASN				89.057	6.886		
	MOTA	1155	C	ASN				91.077	9.328	8.203	1.00 22.08 A
•	MOTA	1156	0	ASN				92.056	9.972	7.864	1.00 20.25 A
4	MOTA	1157	N	ALA				91.170	8.239	8.953	1.00 24.03 A
25	ATOM	1158	CA	ALA				92.464	7.738	9.420	1.00 24.26 A
	MOTA	1159	CB	ALA				92.276	6.502	10.277	1.00 21.70 A
	MOTA	1160	C,	ALA				93.421	7.426	8.296	1.00 24.90 A
	ATOM .	1161	Ο.	ALA				94.615	7.435	8.491	1.00 26.03 A
	MOTA	1162	N	ASP				92.889	7.143	7.108	1.00 25.93 A
30 .	MOTA	1163	CA	ASP	Α	216	••	93.726	6.826	5.963	1.00 26.29 A
	ATOM	1164	CB	ASP	A	216		93.048	5.773	5.091	1.00 32.31 A
	ATOM	1165	CG	ASP	A	216		92.862	4.456	5.812	1.00 38.06 A
	ATOM	1166	OD1	ASP	Α	216		93.780	4.043	6.559	1.00 40.03 A
	ATOM	1167	OD2	ASP	Α	216		91.800	3.823	5.616	1.00 42.79 A
35	ATOM	1168	С	ASP	Α	216		94.046	8.026	5.095	1.00 23.69 A
	ATOM	1169	0	ASP	Α	216		94.717	7.899	4.085	1.00 24.38 A
	ATOM	1170	N	MET	A	217		93.546	9.187	5.478	1.00 21.45 A
	ATOM	1171	ĊA	MET	A	217		93.752	10.418	4.726	1.00 20.48 A
	ATOM	1172	CB	MET	Α	217		95.226	10.614	4.396	1.00 21.48 A
40	ATOM	1173	CG	MET				96.081	10.894	5.629	1.00 21.46 A
	MOTA	1174	SD	MET				95.504	12.311	6.580	1.00 25.32 A
	ATOM	1175	CE	MET				96.079	13.722	5.573	1.00 24.08 A
	ATOM	1176	C	MET	Α	217		92.900	10.556	3.458	1.00 19.63 A
	ATOM	1177	ō	MET				93.245	11.294	2.546	1.00 19.54 A
45	ATOM	1178	N	HIS					9.824	3.405	1.00 18.82 A
73	ATOM	1179	CA	HIS				90.843	9.945	2.311	1.00 18.81 A
	ATOM	1180	CB			218		90.206	8.589	1.994	1.00 20.61 A
	ATOM	1181	CG					91.097	7.666	1.218	1.00 22.68 A
				HIS				91.840	6.605	1.614	1.00 20.37 A
50	ATOM	1182		HIS				91.316	7.806	-0.139	1.00 21.30 A
50	ATOM	1183								-0.541	1.00 20.75 A
	MOTA	1184		HIS				92.153	6.867 6.128	0.501	1.00 20.75 A
	ATOM	1185		HIS				92.485			1.00 20.31 A 1.00 18.97 A
	ATOM	1186	C			218		89.774	10.925	2.863	1.00 16.48 A
c	MOTA	1187	0			218		89.534	10.965	4.083	1.00 18.48 A 1.00 17.41 A
55	ATOM	1188	N			219		89.166	11.721	1.978	1.00 17.41 A
	MOTA	1189	CA			219		88.165	12.702	2.387	
	MOTA	1190	CB			219		87.765	13.695	1.242	1.00 13.43 A
	MOTA	1191		ILE				88.984	14.404	0.698	1.00 10.66 A
	MOTA	1192	CG1	ILE	Α	219		86.973	12.952	0.156	1.00 11.14 A

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	ATOM	. 1193	CD1	ILE	A	219	86.505	13.807	-0.995	1.00 4.26 A
	MOTA	1194	С	ILE	Α	219	86.875	12.067	2.864	1.00 17.14 A
	MOTA	1195	0	ILE	Α	219	86.541	10.943	2.497	1.00 18.77 A
	ATOM	1196	И	GLN	A	220	86.159	12.808	3.696	1.00 17.24 A
5	MOTA	1197	CA	GLN.	Α	220	84.878	12.376	4.203	1.00 18.93 A
	MOTA	1198	CB	GLN	Α	220	85.002	11.756	5.604	1.00 22.02 A
	ATOM	1199	CG	GLN	Α	220	83.791	10.874	5.952	1.00 26.68 A
	ATOM	1200	CD	GLN	Α	220	83.949	10.071	7.253	1.00 31.76 A
	ATOM	1201	OE1	GLN	Α	220	83.437	10.471	8.331	1.00 27.57 A
10	ATOM	1202	NE2	GLN	Α	220	84.667	8.930	7.161	1.00 29.97 A
	ATOM	1203	Ċ			220	84.077	13.652	4.261	1.00 17.44 A
	ATOM	1204	0	GLN	A	220	84.247	14.465	5.170	1.00 17.81 A
	ATOM	1205	N	ILE	Α	221	83.229	13.852	3.263	1.00 15.69 A
	ATOM	1206	CA			221	82.413	15.051	3:230	1.00 16.08 A
15	ATOM	1207	CB			221	81.939	15.359	1.802	1.00 15.82 A
	MOTA	1208	CG2			221		16.519	1.834	1.00 13.95 A
	MOTA	1209	CG1			221	83.163	15.627	0.899	1.00 16.66 A
	ATOM	1210	CD1				82.837	16.045	-0.548	1.00 13.13 A
	ATOM	1211	С			221	81.207	14.892	4.156	1.00 16.52 A
20	ATOM	1212	0			221	80.542	13.860		1.00 16.03 A
:	ATOM	1213	N	THR			80.927	15.922		1.00 17.66 A
	ATOM	1214	CA			222	79.810	15.862	5.882	1.00 17.70 A
	ATOM	1215	CB	THR			80.331	15.433	7.277	1.00 18.71 A
	ATOM	1216	OG1				79.230	15.263	8.172	1.00 16.76 A
25	MOTA	1217	CG2				81.319	16.470	7.825	1.00 16.79 A
-	ATOM	1218	C	THR	Α	222	79.069	17.195	5.980	1.00 17.35 A
	ATOM	1219	0	THR	Α	222	79.246	18.062	5.130	1.00 16.83 A
	MOTA	1220	N	ASP	Α	223	78.244	17.344	7.018	1.00 18.09 A
	ATOM	1221	CA	ASP	Α	223	77.466	18.567	7.268	1.00 19.60 A
30	ATOM	1222	CB	ASP			78.403	19.778	7.311	1.00 22.73 A
	MOTA	1223	CG	ASP			77.763	21.006	7.959	1.00 28.30 A
	MOTA	1224		ASP			76.565	20.931	8.335	1.00 28.17 A
	MOTA	1225	OD2	ASP			78.480	22.042	8.081	1.00 30.99 A
	MOTA	1226	C	ASP			76.382	18.799	6.210	1.00 19.52 A
35	MOTA	1227	0	ASP	Α	223	76.528	19.655	5.340	1.00 19.39 A
	MOTA	1228	N	PHE	A	224	75.283	18.058	6.303	1.00 18.74 A
	MOTA	1229	CA	PHE			74.213	18.168	5.321	1.00 18.81 A
	ATOM	1230	CB	PHE	А	224	73.825	16.773	4.853	1.00 17.07 A
	ATOM	1231	CG	PHE			74.857	16.150	3.971	1.00 17.01 A
40	ATOM	1232		PHE			74.751	16.250	2.578	1.00 16.10 A
	ATOM	1233		PHE			75.982	15.543.	4.521	1.00 14.00 A
	ATOM	1234		PHE			75.761	15.752	1.747	1.00 15.92 A
	ATOM	1235	-	PHE			77.001	15.042	3.699	1.00 15.63 A
4.5	ATOM	1236	CZ	PHE			76.889	15.147	2.309	1.00 15.79 A
45	MOTA	1237	С	PHE			72.997	18.932	5.775	1.00 19.88 A
	ATOM	1238	0	PHE			71.961	18.922	5.115	1.00 19.36 A
	ATOM	1239	N	GLY			73.135	19.599	6.911	1.00 21.38 A
	ATOM	1240	CA	GLY			72.046	20.388	7.439	1.00 21.39 A
	ATOM	1241	С	GLY			71.672	21.545	6.523	1.00 23.43 A
50	ATOM	1242	0	GLY			70.802	22.323	6.869	1.00 26.22 A
	MOTA	1243	N	THR			72.311	21.692	5.370	1.00 22.15 A
	ATOM	1244	CA	THR			71.930	22.784	4.492	1.00 23.85 A
	ATOM	1245	CB	THR			72.986	23.946	4.465	1.00 24.65 A
55	ATOM .	1246		THR			74.197	23.511	3.830	1.00 24.83 A
55	ATOM	1247		THR			73.285	24.420	5.866	1.00 23.67 A
	MOTA	1248	C	THR			71.721	22.289	3.073	1.00 24.12 A
	MOTA	1249	. O	THR			71.646	23.079	2.129	1.00 22.82 A
	MOTA	1250	N	ALA ALA			71.620	20.976	2.935	1.00 23.84 A
	MOTA	1251	CA	HUH	A	221	71.437	20.357	1.637	1.00 26.21 A

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	. ATOM	1252	CB	ALA	A	227	71.774	18.889	1.734	1.00 24.	04 A
	MOTA	1253	С	ALA	A	227	70.026	20.535	1.064	1.00 28.	20 A
	MOTA	1254	0	ALA	Α	227	69.069	20.767	1.801	1.00 29.	29 A
	MOTA	1255	N	ALA	Α	228	69.912	20.449	-0.258	1.00 28.	91 A
5	MOTA	1256	CA	ALA	Α	228	68.623	20.554	-0.928	1.00 31.	02 A
*	MOTA	1257	CB	ALA	Α	228	68.577	21.795	-1.856	1.00 30.	45 A
	MOTA	1258	С	ALA	Α	228	68.501	19.276	-1.745	1.00 32.	
	MOTA	1259	0	ALA	Α	228	69.474	18.846	-2.363	1.00 32.	87 A
	MOTA	1260	N ·	VAL	Α	229	67.328	18.650	-1.732	1.00 32.	95 A
10	MOTA	1261	CA	VAL	A	229	67.126	17.424	-2.503	1.00 34.	26 A
	MOTA	1262	CB	VAL	A	229	66.468	16.347	-1.657	1.00 33.	02 A
	ATOM	1263	CG1	VAL	Α	229	66.194	15.114	-2.498	1.00 33.	80 A
	MOTA	1264	CG2	VAL	A	229	67.356	16.011	-0.496	1.00 31.	38 A
	ATOM	1265	c ·	VAL	Α	229	66.213	17.757	-3.665	1.00 36.	36 A
15	ATOM	1266	0	VAL	Α	229	65.065	18.133	-3.455	1.00 38.	02 A
	MOTA	1267	N	LEU	Α	230	66.715	17.628	-4.889	1.00 37.	75 A
	MOTA	1268	CA	LEU	A	230	65.917	17.965	-6.066	1.00 39.	87 A
	MOTA	1269	ĊВ	LEU	A	230	66.74]	17.775	-7.335	1.00 41.	23 A
	MOTA	1270	CG	LEU	Α	230	68.039	18.585	-7.359	1.00 44.	16 A
20	MOTA	1271	CD1	LEU	Α	230	68.843	18.208	-8.599	1.00 43.	48 A
	ATOM	1272	CD2	LEU	A	230	67.724	20.087	-7.313	1.00 42.	99 A
	MOTA	1273	C	LEU	A	230	64.646	17.137	-6.162	1.00 40.	59 A
	MOTA	1274	0	LEU	Α	230	64.703	15.954	-6.486	1.00 41.	31 A
	ATOM	1275	N	ASN	A	240	65.964	27.756	-2.248	1.00 83.	97 A
25	ATOM	1276	CA	ASN	Α	240	66.333	29.165	-2.370	1.00 84.	48 A
	ATOM	1277	CB	ASN	A	240	65.294	29.907	-3.225	1.00 85.	56 A
•	MOTA	1278	CG	ASN	Α	240	63.949	30.053	-2.524	1.00 86.	.59 A
	ATOM	1279	OD1	ASN	Α	240	63.850	30.682	-1.465	1.00 87.	31 A
	ATOM	1280	ND2	ASN	Α	240	62.904	29.473	-3.115	1.00 86.	.14 A
30	ATOM.	1281	С	ASN	Α	240	66.433	29.828	-0.994	1.00 83.	.85 A
	MOTA	1282	0	ASN	Α	240	66.898	30.963	-0.862	1.00 84.	.11 A
	ATOM	1283	N	ALA	Α	241	65.99	7 29.096	0.023	1.00 83.	.19 A
	ATOM	1284	CA	ALA	Α	241	65.996	5 29.564	1.405	1.00 81	.85 A
	ATOM	1285	С	ALA	Α	241	67.330	29.365	2.127	1.00 79	.97 A
35	ATOM	1286	0	ALA	A	241	67.349	28.777	3.214	1.00 79	.75 A
	ATOM	1287	CB	ALA	Α	241	64.89	28.825	2.183	1.00 85.	.17 A
	MOTA	1288	N	PHE	A	242	68.43	29.850	1.551	1.00 77	.03 A
	ATOM	1289	CA	PHE	A	242	69.73	7 29.680	2.197	1.00 74	.85 A
	ATOM	1290	CB	PHE	Α	242	69.97	28.183	2.438	1.00 73	
40	ATOM	1291	CG	PHE	Α	242	71.31	L 27.861	3.015	1.00 72	.36 A
	ATOM	1292	CD1	PHE	Α	242	71.59	28.116	4.353	1.00 72	.39 A
	MOTA	1293	CD2	PHE	Α	242	72.29	7 27.312	2.210	1.00 72	.03 A
	MOTA	1294	CE1	PHE	Α	242	72.85	27.823	4.879	1.00 72	.87 A
	ATOM	1295	CE2	PHE			73.55		2.714	1.00 72	.25 A
45	ATOM	1296	CZ	PHE	Α	242	73.83	7 27.270	4.054	1.00 72	.96 A
	ATOM	1297	.C	PHE	A	242	70.95	1 30.283	1.462	1.00 73	
	ATOM	1298	0	PHE	A	242	70.95	30.425	0.233	1.00 74	.08 A
	MOTA	1299	N	VAL	A	243	71.97	30.625	2.250	1.00 69	.64 A
	MOTA	1300	CA	VAL	Α	243	73.23	31.204	1.777	1.00 65	.87 A
50	MOTA	1301	CB	VAL	A	243	73.20	7 32.765	1.834	1.00 66	
	MOTA	1302		VAL			74.49		1.271	1.00 65	
	ATOM	1303	CG2	VAL	Α	243	72.00	33.299	1.084	1.00 66	.83 A
	MOTA	1304	C	VAL	Α	243	74.34	30.708	2.703	1.00 62	
	ATOM	1305	0			243	74.47		3.839	1.00 61	
55	MOTA	1306	N			244	75.14		2.204	1.00 57	
	ATOM	1307	CA	GLY	Α	244	76.24		2.967	1.00 51	
	ATOM	1308	C	GLY	Α	244	77.34		3.387	1.00 46	
	MOTA	1309	0			244	77.06		3.757	1.00 48	
	MOTA	1310	N	THR	A	245	78.58	B 29.686	3.325	1.00 42	.06 A

	ATOM	1311	CA	THR A	A 245	79.70	9 30.526	3.726	1.00 36.35 A
	ATOM	1312	CB		A 245	80.92		4.096	1.00 35.76 A
	ATOM	1313	0G1		A 245	. 80.53	_	5.105	1.00 31.66 A
	MOTA	1314	CG2	THR A	A 245		30.534	4.651	1.00 33.72 A
5	ATOM	1315	C		A 245	80.06		2.637	1.00 34.43 A
_	ATOM	1316	ō		A 245	80.30	'	1.485	1.00 33.95 A
	ATOM	1317	N		A 246	80.08		3.034	1.00 32.72 A
	ATOM	1318	CA		A. 246	80.33		2.142	1.00 30.18 A
	ATOM	1319	CB		A 246	80.68		2.952	1.00 30.18 A
10	ATOM	1320	C		A 246	81.37		1.062	1.00 29.56 A
10	ATOM	1321	ō		A 246		9 33.895	-0.113	1.00 30.00 A
	ATOM	1322	N		A 247	82.56	33.242	1.445	1.00 28.03 A
	ATOM	1323	CA		A 247	83.62		0.468	1.00 26.97 A
	ATOM	1324	CB		A 247	84.92		1.182	1.00 28.32 A
15	ATOM	1325	CG		A 247	85.20		2.319	1.00 33.33 A
15	ATOM	1326	CD		A 247	86.60		2.863	1.00 36.16 A
	ATOM	1327		GLN A		87.5		2.335	1.00 36.68 A
	ATOM	1328	NE2		A 247	86.7		3.922	1.00 39.27 A
	ATOM	1329	C		A 247	83.3		-0.583	1.00 25.04 A
20	ATOM	1330	Ö		A 247	83.9		-1.653	1.00 25.92 A
20	ATOM	1331	N		A 248	82.4		-0.304	1.00 22.51 A
	ATOM	1332	CA		A 248	82.1		-1.260	1.00 21.98 A
	ATOM	1333	CB		A 248			-0.541	1.00 17.74 A
	ATOM	1334	CG		A 248	83.6	26 28.444	0.117	1.00 14.83 A
25	ATOM	1335			A 248	84.7	36 28.063	-0.630	1.00 14.53 A
	ATOM '	133.6			A 248	86.0	17 28.034	-0.067	1.00 15.65 A
	MOTA	1337	CD2		A 248	83.8	20 28.784	1.460	1.00 13.57 A
	MOTA	1338	CE2	TYR .	A 248	85.0	86 28.757	2.039	1.00 13.28 A
	MOTA	1339	cz	TYR .	A 248	86.1	92 28.386	1.271	1.00 16.78 A
30	ATOM '	1340	ОН	TYR	A 248	.87.4	71 28.411	1.816	1.00 15.10 A
	MOTA	1341	C	TYR	A 248	80, 8	27 30.091	-2.005	1.00 22.23 A
	ATOM	1342	0	TYR	A 248	80.5	23 29.268	-2.866	1.00 22.78 A
	MOTA	1343	N	VAL	A 249	80.0	54 31.126	-1.680	1.00 21.81 A
	ATOM	1344	CA	VAL	A 249	78.7		-2.308	1.00 22.22 A
35	ATOM	1345	CB	VAL	A 249	78.0		-1.640	1.00 22.82 A
	MOTA	1346			A 249	76.9		-2.496	1.00 22.57 A
	ATOM	1347	CG2		A 249	77.6		-0.243	1.00 22.62 A
	ATOM	1348	C		A 249	78.8		-3.818	1.00 21.92 A
	ATOM	1349	. 0		A 249	79.7		-4.255	1.00 20.01 A
40	ATOM	1350	N		A 250	78.0		-4.609	1.00 22.88 A
	MOTA	1351	CA		A 250	78.0		-6.049	1.00 24.81 A 1.00 25.82 A
	MOTA	1352	CB		A 250	77.3		-6.792 -6.419	1.00 23.02 A 1.00 27.07 A
	MOTA	1353	OG		A 250	75.9	• -		1.00 27.07 A
	MOTA	1354			A 250	77.2		-6.357 -5.582	1.00 25.22 A 1.00 25.88 A
45	MOTA	1355	0		A 250	76.4		-5.582 -7.506	1.00 25.00 A
	MOTA	1356	N		A 251	77.5		-8.495	1.00 27.24 A
	MOTA	1357	CD		A 251	78.6		-7.847	1.00 27.08 A
	MOTA	1358	CA		A 251	76.9 77.6			1.00 25.51 A
	ATOM	1359	CB		A 251	78.1			1.00 27.43 A
50	ATOM	1360	CG		A 251	75.3			1.00 28.00 A
	ATOM	1361	C O		A 251 A 251	74.6			1.00 28.30 A
	ATOM	1362	N		A 251	74.9		•	1.00 28.81 A
	ATOM	1363 1364	CA		A 252	73.4			1.00 29.67 A
55	MOTA MOTA	1365	CB		A 252	73.1			1.00 29.72 A
رر	ATOM	1366	CG		A 252	73.6			1.00 31.04 A
	ATOM	1367	CD		A 252	75.1			1.00 30.61 A
	MOTA	1368			A 252	75.8			1.00 30.55 A
	ATOM	1369			A 252	75.4	134 28.872	-9.130	1.00 30.80 A

	MOTA	1370	C	GLU	Α	252		72.709	33.083	-7.462	1.00 30.83 A
	ATOM	1371	0	GLÜ	Α	252		71.563	33.530	-7.423	1.00 31.87 A
	ATOM	1372	N	LEU	Α	253		73.351	32.639	-6.388	1.00 32.71 A
	ATOM	1373	CA	LEU	A	253		72.734	32.655	-5.073	1.00 33.94 A
5	MOTA	1374	CB	LEU	A	253		73.612	31.901	-4.081	1.00 37.40 A
	ATOM	1375	CG	LEU	Α	253		72.967	31.086	-2.950	1.00 41.64 A
	ATOM	1376	CD1	LEU	Α	253		72.067	31.925	-2.048	1.00 43.86 A
	ATOM	1377	CD2	LEU	Α	253		72.144	30.017	-3.597	1.00 45.52 A
	ATOM	1378	С	LEU	Α	253	•	72.545	34.095	-4.603	1.00 35.67 A
10	ATOM	1379	0	LEU	Α	253		71.589	34.392	-3.897	1.00 37.48 A
	ATOM	1380	N	LEU	Α	254		73.451	34.989	-4.995	1.00 36.38 A
	ATOM	1381	CA	LEU	Α	254		73.372	36.397	-4.600	1.00 36.66 A
	ATOM	1382	CB	LEU	Α	254		74.764	37.032	-4.572	1.00 33.81 A
	ATOM	1383	CG	LEU	A	254		75.824	36.402	-3.674	1.00 33.40 A
15	ATOM	1384	CD1	LEU	Α	254		77.183	37.022	-3.982	1.00 30.48 A
	ATOM	1385	CD2	LEU	Α	254		75.440	36.574	-2.208	1.00 31.43 A
	ATOM	1386	С	LEU	Α	254		72.485	37.240	-5.511	1.00 38.89 A
,	ATOM	1387	0	LEU	Α	254		72.079	38.328	-5.133	1.00 38.85 A
	ATOM	1388	N	THR	Α	255		72.187	36.754	-6.709	1.00 42.60 A
20	MOTA	1389	CA	THR	A	255		71.358	37.528	-7.624	1.00 47.21 A
	MOTA	1390	CB	THR	Α	255		72.102	37.847	-8.941	1.00 47.08 A
	MOTA	1391	OG1	THR	Α	255		72.008	36.718	-9.814	1.00 48.56 A
	ATOM	1392	CG2	THR	A	255		73.581	.38.157	-8.686	1.00 45.65 A
	MOTA	1393	C	THR	A	255		70.044	36.848	-8.009	1.00 51.00 A
25	MOTA	1394	0	THR	Α	255		69.348	37.323	8.903	1.00 51.80 A
	MOTA	1395	N	GLU	A	256	•	69.696	35.745	-7.353	1.00 55.01 A
	MOTA	1396	CA	GLU	Α	256		68.450	35.044	-7.683	1.00 58.97 A
	ATOM	1397	CB	GLU	Ą	256		68.679	34.057	-8.832	1.00 59.81 A
	MOTA	1398	CG	GLU	A	256		68.922	34.707	-10.181	1.00 63.59 A
30	MOTA	1399	CD	GLU	Α	256		69.343	33.707	-11.240	1.00 65.64 A
	ATOM	1400 -		GLU				68.727	32.617	-11.310	1.00 67.44 A
	MOTA	1401	OE2	GLU	Α	256		70.285	34.015	-12.007	1.00 66.61 A
	MOTA	1402	C	GLU	Α	256		67.859	34.279	-6.512	1.00 60.83 A
	ATOM	1403	0	GLU	A	256	-	66.701	33.861	-6.563	1.00 61.27 A
35	MOTA	1404	N	ALA				68.657	34.100	-5.463	1.00 62.31 A
	MOTA	1405	CA	ALA	Α	257	. •	68.234	33.348	-4.285	1.00 63.29 A
	MOTA	1406	CB	ALA	A	257		66.867	33.847	-3.784	1.00 62.76 A
	MOTA	1407	C	ALA	Α	257		68.157	31.860	-4.651	1.00 63.64 A
	ATOM	1408	0	ALA				67.790	31.028	-3.825	1.00 64.96 A
40 -	MOTA	1409	N	ŞER	A	258		68.523	31.532	-5.888	1.00 62.79 A
	MOTA	1410	CA	SER				68.485	30.150	-6.378	1.00 62.30 A
	ATOM	1411	CB	SER	A	258		68.049	30.144	-7.847	1.00 63.00 A
	ATOM	1412	OG	SER				68.762	31.129	-8.582	1.00 63.40 A
	MOTA	1413	C	SER				69.816	29.402	-6.237	1.00 61.09 A
45	ATOM	1414	0	SER				70.862	30.009	-6.009	1.00 62.12 A
	MOTA	1415	N	ALA				69.774	28.083	-6.389	1.00 58.47 A
	MOTA	1416	CA	ALA				70.979	27.270	-6.278	1.00 55.79 A
	ATOM	1417	CB	ALA				71.403	27.164	-4.837	1.00 56.24 A
	ATOM	1418	C	ALA				70.738	25.886	-6.842	1.00 53.38 A
50	MOTA	1419	0	ALA				69.641	25.347	-6.736	1.00 54.10 A
	MOTA	1420	N	CYS			-	71.768	25.302	-7.433	1.00 49.75 A
	MOTA	1421	CA	CĂR				71.623	23.988	-8.015	1.00 45.68 A
	MOTA	1422	CB	CYS				71.067	24.106	-9.438	1.00 48.50 A
	MOTA	1423	SG	CYS				69.936	22.732	-9.899	1.00 57.53 A
55	MOTA	1424	C	CYS				72.980	23.318	-8.022	1.00 41.30 A
	MOTA	.1425	0	CYS					23.762	-7.335	1.00 39.24 A
	MOTA	1426	N	LYS				73.118	22.258	-8.805	1.00 36.63 A
	ATOM	1427	CA	LYS				74.369	21.535	-8.866	1.00 33.81 A
	ATOM	1428	CB	LYS	A	261		74.261	20.416	-9.897	1.00 34.27 A

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•	ATOM	1429	CG	LYS	А	261	73.250	19.362	-9.488	1.00 34.04 A
-	ATOM	1430	CD	LYS	Α	261	72.995	18.353	-10.577	1.00 33.10 A
	ATOM	1431	CE	LYS			71.983	17.336	-10.105	1.00 32.48 A
	ATOM	1432	NZ	LYS			71.660	16.357	-11.176	1.00 33.10 A
5	ATOM	1433	C	LYS			75.565	22.419	-9.153	1.00 31.80 A
-	ATOM	1434	ō	LYS			76.636	22.214	-8.589	1.00 31.89 A
	ATOM	1435	N	SER			75.389	23.405	-10.025	1.00 29.92 A
-	ATOM	1436	CA	SER			76.477		-10.354	1.00 28.19 A
	ATOM	1437	CB	SER			76.034		-11.417	1.00 29.90 A
10	ATOM	1438	OG	SER			76.184		-12.695	1.00 34.45 A
10		1439	C	SER			77.047	25.069	-9.155	1.00 25.77 A
	ATOM		0	SER			78.225	25.405	-9.146	1.00 26.59 A
•	ATOM	1440		SER			76.216	25.347	-8.159	1.00 23.42 A
	ATOM	1441	N	SER				26.040	-6.953	1.00 23.12 H
15	ATOM	1442	CA				76.663	26.209	-5.979	1.00 24.64 A
15	ATOM	1443	CB	SER			75.502		-6.572	1.00 24.04 A 1.00 31.12 A
	ATOM	1444	OG	SER			74.463	26.963		1.00 31.12 A 1.00 21.37 A
	ATOM	1445	Ċ	SER			77.777	25.233	-6.283	
	ATOM	1446	0	SER			78.745	25.803	-5.788	1.00 20.74 A
	MOTA	1447	N	ASP			77.640	23.909	-6.268	1.00 19.11 A
20	ATOM	1448	CA	ASP			78.674	23.062	-5.682	1.00 19.35 A
	ATOM	1449	CB	ASP			78.206	21.609	-5.579	1.00 18.45 A
	MOTA	1450	CG	ASP		•	77.164	21.406	-4.500	1.00 19.39 A
	ATOM	1451		ASP			76.998	22.304	-3.649	1.00 20.34 A
	MOTA	1452		ASP			76.522	20.338	-4.488	1.00 19.48 A
25	MOTA	1453	C	ASP			79.943	23.127	-6.542	1.00 19.34 A
	ATOM	1454 _.	0	ASP			81.052	23.147	-6.018	1.00 20.70 A
	MOTA	1455	N	LEU			79.772	23.162	-7.864	1.00 17.68 A
	MOTA	1456	CA	LEU			80.898	23.232	-8.774	1.00 17.42 A
	ATOM	1457	CB	LEU			80.406		-10.208	1.00 19.36 A
30	MOTA	1458	CG	LEU			79.683		-10.453	1.00 19.53 A
	MOTA	1459		LEU		•	79.189	21.655	-11.879	1.00 17.18 A
	MOTA	1460		LEU			80.625		-10.168	1.00 14.91 A
	MOTA	1461	C	LEU	А	265	81.619	24.566	-8.600	1.00 19.06 A
	MOTA	1462	0	LEU	Α	265	82.850	24.649	-8.697	1.00 18.60 A
35	MOTA	1463	N	TRP	Α	266 .	80.853	25.621	-8.350	1.00 18.60 A
	MOTA	1464	CA	TRP	Α	266	81.468	26.902	-8.107	1.00 18.62 A
	ATOM	1465	CB	TRP	A	266	80.405	27.976	-7.876	1.00 19.75 A
	MOTA	1466	CG	TRP	Α	266	80.997	29.277	-7.382	1.00 21.53 A
	ATOM	1467	CD2	TRP	А	266	81.357	30.420	-8.174	1.00 22.40 A
40	ATOM	1468	CE2	TRP			81.917	31.375	-7.296	1.00 22.70 A
	ATOM	1469	CE3	TRP	A	266	81.260	,30.728	-9.541	1.00 21.62 A
	MOTA	1470	CD1	TRP	Α	266	81.344	29.582	-6.094	1.00 20.15 A
	MOTA	1471	NE1		A	266	81.896	30.835	-6.037	1.00 20.80 A
	ATOM	1472	CZ2	TRP	Α	266	82.382	32.624	-7.739	1.00 22.47 A
45	MOTA	1473	CZ3	TRP	Α	266	81.721	31.961	-9.981	1.00 22.48 A
	MOTA	1474		TRP			82.276	32.898	-9.080	1.00 23.40 A
	MOTA	1475	С	TRP	Α	266	82.338	26.734	-6.857	1.00 18.89 A
	ATOM	1476	0	TRP	Α	266	83.523	27.070	-6.875	1.00 20.01 A
	ATOM	1477	N	ALA	А	267	81.755 .	26.204	-5.780	1.00 16.09 A
50	ATOM	1478	CA	ALA	Α	267	82.502	25.994	-4.540	1.00 15.55 A
	MOTA	1479	CB	ALA	Α	267	81.630	25.313	-3.499	1.00 13.20 A
	MOTA	1480	C	ALA	Α	267	83.738	25.145	-4.813	1.00 16.44 A
	MOTA	1481	0	ALA	A	267	84.802	25.345	-4.218	1.00 17.65 A
	ATOM	1482	N	LEU	A	268	83.597	24.181	-5.710	1.00 15.96 A
55	MOTA	1483	CA	LEU	A	268	84.732	23.336	-6.055	1.00 17.56 A
	ATOM	1484	CB	LEU	Α	268	84.315	22.281	-7.098	1.00 16.91 A
	ATOM	1485	CG	LEU	Α	268	85.477	21.535	-7.775	1.00 16.43 A
	ATOM	1486	CD1	LEU	Α	268	86.214	20.697	-6.766	1.00 ·15.17 A
	MOTA	1487	CD2	LEU	A	268	84.947	20.643	~8.871	1.00 17.18 A
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	ATOM	1488	C	LEU	Α	268		85.892	24.193	-6.599	1.00 15.96 A
	ATOM	1489	0	LEU	A	268		87.032	24.040	-6.178	1.00 14.54 A
	MOTA	1490	N	GLY	Α	269		85.578	25.092	7.530	1.00 17.15 A
	ATOM	1491	CA	GLY	Α	269		86.590	25.957	-8.116	1.00 18.32 A
5	ATOM	1492	C	GLY				87.339	26.722	-7.042	1.00 19.39 A
_	ATOM	1493	ō	GLY				88.579	26.777	-7.042	1.00 19.66 A
	MOTA	1494	N	CÝS				86.579	27.297	-6.111	1.00 17.50 A
	MOTA		CA	CYS				87.154	28.043	-5.010	1.00 17.72 A
	ATOM	1496	СВ	CYS				86.047	28.551	-4.088	1.00 18.96 A
10	ATOM	1497	SG	CYS				84.981	29.801	-4.798	1.00 19.62 A
10			C	CYS				88.114	27.182	-4.201	1.00 18.63 A
•	ATOM	1498	0	CYS				89.213	27.612	-3.850	1.00 18.78 A
	ATOM	1499 1500		ILE				87.679	25.962	-3.900	1.00 20.05 A
	ATOM		N						25.019	-3.130	1.00 20.03 A
1.5	ATOM	1501	CA	ILE				88.479			1.00 20.00 A
15	MOTA	1502	CB	ILE				87.668	23.755		
	ATOM	1503		ILE				88.592	22.654	-2.302	1.00 18.31 A
	ATOM	1504		ILE				86.558	24.104	-1.810	1.00 18.38 A
	MOTA	1505		ILE				85.396	23.125	-1.783	1.00 14.68 A
	MOTA	1506	С	ILE				89.761	24.629	-3.858	1.00 20.41 A
20	ATOM	1507 ·	0	ILE				90.826	24.548	-3.234	1.00 21.81 A
	ATOM	1508	N	ILE	A	272		89.669	24.398	-5.166	1.00 18.41 A
	MOTA	1509	CA	ILE		-		90.860	24.035	-5.934	1.00 19.20 A
	ATOM .	1510	CB	ILE	Α	272		90.526	23.730	-7.412	1.00 20.04 A
	MOTA	1511	CG2	ILE	Α	272		91.808	23.488	-8.199	1.00 17.73 A
25 -	MOTA	1512	CG1	ILE	А	272		89.602	22.523	-7.513	1.00 19.47 A
	MOTA	1513	CD1	ILE	А	272		89.001	22.386	-8.872	1.00 20.31 A
	MOTA	1514	С	ILE	A	272		91.858	25.191	-5.932	1.00 19.57 A
	MOTA	1515	0	ILE	Α	272		93.061	24.978	-5.884	1.00 20.97 A
	ATOM	1516	N	TYR	Α	273		91.338	26.413	-6.028	1.00 19.42 A
30	ATOM	1517	CA	TYR	Α	273		92.157	27.606	-6.041	1.00 18.41 A
•	ATOM	1518	СВ	TYR	Α	273		91.272	28.826	-6.294	1.00 18.70 A
	ATOM	1519	CG	TYR	Α	273		91.998	30.147	-6.252	1.00 19.81 A
	ATOM	1520	CD1	TYR	Α	273		92.357	30.729	-5.035	1.00 21.25 A
•	ATOM	1521	CE1	TYR	Α	273		93.072	31.936	-4.990	1.00 22.12 A
35	ATOM	1522	CD2	TYR	Α	273		92.366	30.804	-7.433	1.00 20.45 A
	ATOM	1523	CE2	TYR	A	273		93.081	32.005	-7.403	1.00 20.42 A
	ATOM	1524	CZ			273		93.432	32.563	-6.178	1.00 23.33 A
	ATOM	1525	ОН			273		94.159	33.731	-6.138	1.00 23.26 A
	ATOM	1526	С	TYR	Α	273		92.848	27.699	-4.687	1.00 19.40 A
40	MOTA	1527	ō			273		94.051	27.945	-4.598	1.00 19.44 A
. •	ATOM	1528	N			274		92.079	27.471	-3.632	1.00 19.53 A
	ATOM	1529	CA			274		92.602	27.517	-2.278	1.00 21.26 A
	ATOM	1530	CB			274		91.450	27.399	-1.290	1.00 22.36 A
	ATOM	1531	CG			274		91.838	27.629		1.00 21.87 A
45	ATOM	1532	CD			274		90.643	27.531	1.054	1.00 23.64 A
73	ATOM	1533		GLN				89.499	27.479	0.585	1.00 22.12 A
	ATOM	1534		GIM				90.890	27.517	2.369	1.00 24.45 A
	ATOM	1535	C			274	• .	93.656	26.435	-1.980	1.00 22.20 A
•	ATOM	1536				274		94.549		-1.160	1.00 22.03 A
50	ATOM	1536	и О			275		93.558	25.275	-2.625	1.00 21.82 A
JU	ATOM					275	į.	94.550	24.223	-2.385	1.00 21.02 A
		1538	CA							-3.015	1.00 21.33 A
	ATOM	1539	CB			275		94.104 92.934	22.886	-2.341	1.00 19.15 A
	ATOM	1540	CG			275			22.153	-2.341	1.00 19.79 A
<i>E F</i>	MOTA	1541		LEU				92.528	20.915		1.00 15.75 A 1.00 16.56 A
55	ATOM	1542		LEU		_		93.333	21.757	-0.938	1.00 10.50 A 1.00 21.62 A
	ATOM	1543	C			275		95.910	24.630	-2.962	1.00 21.02 A 1.00 21.98 A
	ATOM	1544	0			275		96.950	24.414	-2.353	1.00 21.38 A
	ATOM	1545	N			276	-	95.884	25.239	-4.137	1.00 20.34 A 1.00 21.48 A
	ATOM	1546	CA	VAL	A	276		97.095	25.639	-4.828	1.00 21.40 A

			~		0.00			c	
	MOTA	1547	CB	VAL A		96.810	25.795	-6.338	1.00 21.76 A
	ATOM	. 1548		VAL A		98.035	26.269	-7.061	1.00 20.72 A
	MOTA	1549	CG2	VAL A		96.332	24.479	-6.908	1.00 21.98 A
	ATOM	1550	C	VAL A		97.696	26.946	-4.315	1.00 23.17 A
5	ATOM	1551	0	VAL A	276	98.913	27.055	-4.141	1.00 24.82 A
	ATOM	1552	N	ALIA A	277	96.837	27.934	-4.085	1.00 22.20 A
	ATOM	1553	CA	ALA A	277	97.271	29.230	-3.628	1.00 19.31 A
	ATOM	1554	ĊВ	ALA A	277	96.339	30.293	-4.174	1.00 19.24 A
	ATOM	1555	C	ALA A		97.380	29.350	-2.113	1.00 20.10 A
10	ATOM	1556	ō	ALA A		98.096	30.222	-1.622	1.00 20.73 A
	ATOM	1557	N	GLY A		96.686	28.493	-1.368	1.00 19.16 A
	ATOM	1558	CA	GLY A		96.748	28.579	0.084	1.00 13.10 A 1.00 18.62 A
	ATOM	1559	C	GLY A		95.634	29.425	0.677	
						95.462			•
1.5	ATOM	1560	0	GLY A			29.483	1.903	1.00 20.36 A
15	ATOM	1561	N	LEU A		94.865	30.084	-0.190	1.00 22.58 A
	ATOM	1562	CA	LEU A		93.742	30.917	0.254	1.00 24.03 A
	MOTA	1563	CB	LEU A		94.190	32.365	0.448	1.00 23.98 A
	ATOM	1564	CG	LEU A		95.322	32.744	1.396	1.00 25.93 A
	ATOM	1565		LEU A		95.622	34.215	1.140	1.00 25.95 A
20	ATOM	1566	CD2	LEU A	279	94.950	32.511	2.873	1.00 24.23 A
•	MOTA	1567	C	LEÙ A	279	92.575	30.940	-0.735	1.00 23.96 A
	ATOM	1568	0	LEU A	279	92.759	30.776	-1.939	1.00 23.93 A
	MOTA	1569	N	PRO A	280	91.353	31.151	-0.231	1.00 24.60 A
	ATOM	1570	CD	PRO A	280	90.987	31.360	1.185	1.00 23.93 A
25	ATOM	1571	CA	PRO A	280	90.177	31.208	-1.109	1.00 24.56 A
	ATOM	1572	СВ	PRO A		89.024	31.319	-0.116	1.00 24.33 A
	ATOM	1573	CG	PRO A		89.656	32.027	1.076	1.00 24.23 A
	ATOM	1574	C	PRO A		90.324	32.453	-2.033	1.00 25.82 A
	ATOM	1575	ō	PRO A		90.892	33.458	-1.632	1.00 27.28 A
30	ATOM	1576	N	PRO A		89.798	32.396	-3.268	1.00 25.40 A
50	ATOM	1577	CD	PRO A		88.807	31.385	-3.660	1.00 25.40 A
				PRO A				-4.272	1.00 24.99 A
	ATOM	1578	CA			89.862 89.150	33.470		
	ATOM	1579	CB	PRO A			32.871	-5.489	1.00 24.76 A
26	ATOM	1580		PRO A		88.882	31.442	-5.137	1.00 26.48 A
35	ATOM	1581	C	PRO A		89.254	34.836	-3.921	1.00 25.24 A
	ATOM	1582	0	PRO A		89.803	35.886	-4.272	1.00 25.07 A
	MOTA	1583	Ŋ	PHE A		88.103	34.821	-3.264	1.00 24.47 A
	MOTA	1584	CA	PHE A		87.435	36.059	-2.918	1.00 24.29 A
	ATOM	1585	CB	PHE A		85.964	35.961	-3.320	1.00 23.11 A
40	ATOM	1586	CG	PHE A		85.759	35.596	-4.774	1.00 21.99 A
-	MOTA	1587		PHE A		85.936	36.543	-5.775	1.00 20.97 A
	ATOM	1588		PHE A		85.448	34.285	-5.139	1.00 21.76 A
	MOTA	1589		PHE A		85.812	36.194	-7.124	1.00 20.59 A
	MOTA	1590	CE2	PHE A		85.325	33.923	-6.469	1.00 20.98 A
45	MOTA	1591	CZ	PHE A	282	85.509	34.885	-7.471	1.00 23.01 A
	ATOM	1592	C	PHE A	282	87.579	36.366	-1.435	1.00 25.85 A
•	ATOM	1593	0	PHE A	282	86.963	35.707	-0.596	1.00 27.04 A
	MOTA	1594	· N	ARG A	283	88.414	37.358	-1.124	1.00 27.56 A
	ATOM	1595	CA	ARG A		88.676	37.784	0.260	1.00 27.41 A
50	ATOM	1596	CB	ARG A		90.116	37.451	0.648	1.00 28.05 A
	ATOM	1597	CG	ARG A		90.523	36.020	0.327	1.00 32.73 A
	ATOM	1598	CD	ARG A		91.944	35.722	0.788	1.00 36.54 A
	ATOM	1599	· NE	ARG A		92.942	36.490	0.043	1.00 39.92 A
	ATOM	1600	CZ	ARG A		93.202	36.329	-1.253	1.00 33.52 A
55	ATOM	1600		ARG A		92.544	35.421	-1.255	1.00 42.59 A
55	ATOM							-1.853	1.00 43.94 A
		1602	NH2			94.112	37.090		1.00 43.94 A 1.00 27.01 A
	ATOM	1603	C	ARG A		88.445	39.291	0.394	
	ATOM	1604	0	ARG A		88.682	40.047	-0.557	1.00 26.54 A
	ATOM	1605	N	ALA A	204	87.977	39.724	1.568	1.00 26.05 A

	ATOM	1606	CA	ALA	A	284		87.694	41.135	1.812	1.00 23.42 A
	ATOM	1607	CB	ALA	Α	284		86.529	41.579	0.967	1.00 21.82 A
	MOTA	1608	C	ALA	A	284		87.386	41.383	3.280	1.00 24.72 A
	ATOM	1609	0	ALA	Α	284		87.193	40.440	4.048	1.00 24.83 A
5	MOTA	1610	N	GLY	A	285		87.330	42.663	3.659	1.00 25.04 A
	MOTA	1611	CA	GLY	Α	285		87.055	43.039	5.035	1.00 23.67 A
	ATOM	1612	C	GLY	A	285		85.761	42.542	5.652	1.00 25.13 A
	MOTA	1613	0	GLY	Α	285	•	85.718	42.302	6.855	1.00 26.60 A
	MOTA	1614	N	ASN	A	286		84.700	42.399	4.862	1.00 24.84 A
10	ATOM	1615	CA	ASN	А	286		83.418	41.923	5.391	1.00 23.82 A
	ATOM	1616	CB	ASN	Α	286		82.567	43.098	5.899	1.00 23.66 A
	ATOM	1617	CG	ASN	A	286		82.362	44.190	4.843	1.00 24.14 A
	MOTA	1618	OD1	ASN	Α	286		81.835	43.947	3.747	1.00 22.27 A
	ATOM	1619	ND2	ASN	Α	286		82.776	45.402	5.178	1.00 24.49 A
15	MOTA	1620	C	ASN	Α	286		82.672	41.185	4.296	1.00 24.75 A
	ATOM	1621	0	ASN	A	286		83.124	41.160	3.153	1.00 25.32 A
•	ATOM	1622	N	GLU	A	287		81.522	40.610	4.630	1.00 26.04 A
	ATOM	1623	CA	GLU	A	287		80.746	39.865	3.641	1.00 27.47 A
	ATOM	1624	CB	GLU	Α	287		79.549	39.175	4.287	1.00 30.33 A
20	ATOM	1625	CG	GLU	Α	287		79.935	38.202	5.364	1.00 36.51 A
	ATOM	1626	CD	GLU	A	287		78.792	37.288	5.766	1.00 41.45 A
	ATOM	1627	OE1	GLU	Α	287		77.608	37.712	5.641	1.00 43.02 A
	MOTA	1628	OE2	GLU	Α	287		79.092	36.155	6.222	1.00 41.33 A
	ATOM	1629	C	GLU	A	287		80.250	40.679	2.467	1.00 25.95 A
25	MOTA	1630	0	GLU	A	287	•	80.279	40.203	1.330	1.00 25.67 A
	ATOM	1631	N	TYR	Α	288		79.772	41.893	2.730	1.00 25.20 A
	ATOM	1632	CA	TYR	Α	288		79.276	42.731	1.644	1.00 22.91 A
	ATOM	1633	CB	TYR	Α	288		78.870	44.113	2.152	1.00 22.98 A
	MOTA	1634	CG	TYR	Α	288		78.459	45.068	1.038	1.00 23.01 A
30	ATOM	1635	CD1	TYR				77.166	45.031	0.478	1.00 24.16 A
	ATOM	1636	CE1					76.814	45.869	-0.589	1.00 22.73 A
	ATOM	1637	CD2	TYR				79.376	45.965	0.508	1.00 21.34 A
	ATOM	1638	CE2	TYR				79.043	46.796	-0.551	1.00 23.71 A
	ATOM	1639	CZ	TYR				77.771	46.748	-1.099	1.00 25.48 A
35	ATOM	1640	ОН	TYR				77.490	47.571	-2.172	1.00 26.98 A
	ATOM	1641	С	TYR				80.352	42.882	0.578	1.00 22.37 A
	ATOM	1642	0	TYR				80.068	42.735	-0.603	1.00 22.65 A
	ATOM	1643	N	LEU				81.590	43.155	0.993	1.00 22.04 A
40	ATOM	1644	CA	ĻEU				82.691	43.326	0.037	1.00 23.92 A
40	ATOM	1645	CB	LEU				83.927	43.907	0.748	1.00 21.71 A
	ATOM	1646	CG	LEU				83.661	45.326	1.298	1.00 23.89 A
	ATOM	1647		LEU				84.716	45.787	2.326	1.00 17.24 A
	ATOM	1648		LEU				83.570	46.273	0.118	1.00 19.08 A
4.5	ATOM	1649	C	LEU				83.050	42.025	-0.693	1.00 24.50 A
45	MOTA	1650	0	LEU				83.446	42.042	-1.852	1.00 24.85 A
	ATOM	1651	N	ILE				82.906	40.904	-0.002	1.00 24.71 A
	ATOM	1652	CA	ILE				83.182	39.601	-0.570	1.00 25.86 A
	ATOM	1653	CB	ILE				83.131	38.521	0.528	1.00 26.67 A
50	ATOM	1654		ILE				83.229	37.154	-0.087	1.00 27.57 A
50	ATOM	1655		ILE				84.282	38.736	1.511	1.00 28.90 A
	MOTA	1656				290.		84.173	37.928	2.798	1.00 28.83 A 1.00 26.89 A
	ATOM	1657	C	ILE				82.127	39.303	-1.637	
	MOTA	1658	0	ILE				82.446	38.879	-2.757	1.00 26.18 A
55	MOTA	1659	N	PHE				80.864	39.531	-1.294	1.00 27.48 A 1.00 28.46 A
55	MOTA	1660	CA'	PHE				79.789	39.287	-2.249 ⁻	1.00 28.46 A
	MOTA	1661	CB	PHE		291	•	78.434	39.587	-1.620 -0.496	1.00 27.24 A 1.00 27.02 A
	ATOM	1662	CG	PHE				78.079	38.664		
	ATOM ·	1663		PHE				78.716	37.431	-0.365 0.399	1.00 26.90 A 1.00 25.83 A
	ATOM	1664	CDZ	LUE	~	2 J L		77.074	38.996	U.333	1.00 23.03 A

36.545 78.353 0.637 1.00 27.02 A MOTA 1665 CE1 PHE A 291 1.00 28.02 A 76.700 38.109 ATOM 1666 CE2 PHE A 291 1.412 PHE A 291 77.338 36.882 1.532 1.00 26.74 A MOTA 1667 CZ79.971 1.00 29.11 A MOTA 1668 С PHE A 291 40.159 -3.467 -4.584 1.00 30.18 A 79.595 39.787 ATOM 1669 0 PHE A 291 GLN A 292 80.559 41.324 -3.240 1.00 28.88 A 1670 ATOM N 42.280 1671 GLN A 292 80.783 -4.304 1.00 30.00 A ATOM CA 81.215 43.604 -3.679 1.00 32.57 A ATOM 1672 CB GLN A 292 44.799 -4.599 1.00 35.12 A 1673 GLN A 292 81.191 ATOM CG -3.817 1.00 38.65 A 10 MOTA 1674 CD GLN A 292 81.208 46.113 82.159 46.409 -3.078 1.00 39.67 A 1675 OE1 GLN A 292 ATOM 46.903 -3.972 1.00 38.94 A 1676 NE2 GLN A 292 80.150 ATOM MOTA 1677 С GLN A 292 81.822 41.755 -5.296 1.00 28.96 A -6.510 1.00 28.45 A 41.844 ATOM 1678 GLN A 292 81.633 0 41.193 -4.787 1.00 26.32 A LYS A 293 82.910 15 MOTA 1679 N 40.661 1680 LYS A 293 83.930 -5.669 1.00 26.90 A ATOM CA -4.858 1.00 28.03 A CB LYS A 293 85.174 40.319 MOTA 1681 85.777 41.539 -4.177 1.00 28.52 A ATOM 1682 CG LYS A 293 1683 LYS A 293 87.065 41.208 -3.482 1.00 29.14 A ATOM CD 1.00 30.09 A 87.912 42.449 -3.269 20 ATOM 1684 CE LYS A 293 LYS A 293 89.165 42.157 -2.490 1.00 30.06 A 1685 NZ MOTA 1686 LYS A 293 83.414 39.432 -6.434 1.00 26.13 A ATOM C LYS A 293 83.721 39.231 -7.617 1.00 26.02 A ATOM 1687 0 -5.755 1.00 24.49 A ATOM 1688 N ILE A 294 82.617 38.621 1.00 24.40 A 25 ILE A 294 82.047 37.429 -6.362 MOTA 1689 CA 36.680 ~5.340 1.00 23.24 A 1690 ILE A 294 81.168 ATOM CB 1691 -6.046 1.00 21.00 A ATOM CG2 ILE A 294 80.154 35.763 CG1 ILE A 294 82.072 35.929 -4.365 1.00 19.23 A ATOM 1692 -3.067 1.00 17.91 A 81.388 35.559 ATOM 1693 CD1 ILE A 294 ILE A 294 -7.608 1.00 26.38 A 81.224 37.744 30 1694 С MOTA ATOM 1695 O ILE A 294 81.428 37.139 -8.661 1.00 25.96 A MOTA 1696 N ILE A 295 80.303 38.694 -7.505 1.00 28.38 A -8.659 ATOM 1697 CA ILE A 295 79.467 39.018 1.00 31.11 A ILE A 295 78.243 39.852 -8.248 1.00 31.46 A MOTA 1698 CB 39.181 .CG2 ILE A 295 -7.068 1.00 32.78 A 35 1699 77.548 ATOM -7.871 1.00 31.79 A 1700 CG1 ILE A 295 78.669 41.268 ATOM MOTA 1701 CD1 ILE A 295 77.518 42.132 -7.438 1.00 33.46 A 1.00 31.35 A MOTA 1702 C ILE A 295 80.201 39.731 -9.798 ILE A 295 39.784 -10.930 1.00 32.03 A 79.709 MOTA 1703 0 40 1704 N LYS A 296 81.374 40.269 -9.511 1.00 30.68 A ATOM LYS A 296 40.937 -10.552 1.00 31.64 A 1705 CA 82.129 ATOM 1.00 32.01 A LYS A 296 82.683 42.275 -10.041 MOTA 1706 CB MOTA 1707 CG LYS A 296 81.605 43.213 -9.520 1.00 34.12 A LYS A 296 -8.841 1.00 37.38 A 44.441 ATOM 1708 CD 82.184 -9.803 1.00 40.30 A 45 1709 CE LYS A 296 82.299 45.609 MOTA ATOM 1710 NZ LYS A 296 82.864 46.819 -9.119 1.00 42.94 A 40.010 -10.966 1.00 31.87 A LYS A 296 1711 C 83.258 ATOM LYS A 296 40.398 -11.745 1.00 32.98 A 0 84.135 ATOM 1712 1713 N **LEU A 297** 83.227 38.780 -10.443 1.00 30.62 A MOTA LEU A 297 37.775 -10.735 1.00 29.78 A 50 CA 84.253 ATOM 1714 **LEU A 297** 84.100 37.253 -12.169 1.00 29.42 A ATOM 1715 CB 35.931 -12.527 1.00 29.13 A 1716 CG **LEU A 297** 84..802 MOTA 34.776 -11.783 1.00 27.91 A CD1 LEU A 297 84.142 ATOM 1717 CD2 LEU A 297 84.725 35.682 -14.024 1.00 26.86 A 1718 ATOM 38.436 -10.565 55 1719 C **LEU A 297** 85.622 1.00 29.62 A ATOM 1.00 28.99 A 38.333 -11.419 0 LEU A 297 86.489 MOTA 1720 N GLU A 298 39.091 -9.427 1.00 29.81 A 85.807 ATOM 1721 -9.143 1.00 30.88 A **GLU A 298** 87.027 39.826 ATOM 1722 CA 41.166 ATOM 1723 CB **GLU A 298** 86.622 -8.510 1.00 33.22 A

	ATOM	1724	CG	GLU A 29	87.754	42.136	-8.228	1.00	38.19	4
	ATOM	1725	CD	GLU A 29	87.317	43.274	-7.303		41.34	
	ATOM	1726	OE1	GLU A 29	86.416	44.054	-7.684		43.93	
	ATOM	1727	OE2	GLU A 29	87.867	43.382	-6.187		43.19	
5	ATOM	1728	C	GLU A 29	88.071	39.110	-8.269		29.28	
_	ATOM	1729	0	GLU A 29	88.066	39.230	-7.045		30.04	
	ATOM	1730	N	TYR A 29	9 88.972	38.375	-8.906		26.46	
	ATOM	1731	CA	TYR A 29	90.034	37.669	-8.194	1.00	26.46	A
	MOTA	1732	CB	TYR A 29	9 89.548	36.315	-7.640		24.23	
10	ATOM	1733	CG	TYR A 29	9 89.403	35.252	-8.709	1.00	23.32	A
	ATOM	1734	CD1	TYR A 29	9 88.369	35.318	-9.653	1.00	23.42	A
	ATOM	1735		TYR A 29		34.392	-10.686		23.13	
	ATOM	1736	CD2	TYR A 29	9 90.337	34.227	-8.829	1.00	21.77	A
	ATOM	1737	CE2	TYR A 29	9 90.250	33.292	-9.864	1.00	21.81	A
15	MOTA	1738	CZ	TYR A 29	9 89.214		-10.784	1.00	22.35	A
	ATOM	1739	OH	TYR A 29	9 89.089	32.444	-11.780	1.00	21.61	A
	ATOM	1740	C	TYR A 29		37.416	-9.245	1.00	28.31	A
	ATOM	1741	0	TYR A 29		37.622	-10.426	1.00	27.25	A
	ATOM	1742	N	ASP A 30	0 92.277	36.959	-8.844	1.00	30.57	A
20	ATOM	1743	CA	ASP A 30		36.687	-9.851	1.00	33.57	Α
. 20	ATOM	1744	СВ	ASP A 30		37.980	-10.193	1.00	38.77	Α
	ATOM	1745	CG	ASP A 30		38.768	-8.968	1.00	43.17	A
	ATOM	1746		ASP A 30		38.283	-8.197	1.00	46.59	Α
	ATOM	1747		ASP A 30		39.865	-8.773	1.00	45.78	Α
25	ATOM	1748	Ċ	ASP A 30		35.607	-9.364		33.20	
23	ATOM	1749	o	ASP A 30		35.354	-8.169	1.00	33.46	A
	ATOM	1750	N	PHE A 30		34.959	-10.287		32.16	
	MOTA	1751	CA	PHE A 30		33.892	-9.910	1.00	33.41	A
	ATOM	1752	СВ	PHE A 30		32.813	-11.001	1.00	32.89	Α
30	ATOM	1753	CG	PHE A 30		32.240	-11.403		33.05	
50	ATOM	1754		PHE A 30		32.921	-12.297		31.61	
	ATOM	1755		PHE A 30		31.006	-10.905		30.94	
	ATOM	1756		PHE A 30		32.387	-12.687	1.00	31.29	A
	ATOM	1757		PHE A 30		30.466	-11.287		31.42	
35	ATOM	1758	CZ	PHE A 30	_	31.157	-12.184	1.00	32.69	Α.
55	ATOM	1759	C	PHE A 30		34.359	-9.649	1.00	34.23	Α
	ATOM	1760	ō	PHE A 30		35.274	-10.303	1.00	33.66	Α
	ATOM	1761	N	PRO A 30		33.750	-8.665	1.00	35.45	Α
	ATOM	1762	CD	PRO A 30		32.932	-7.564	1.00	35.55	A
40	ATOM	1763	CA.	PRO A 30		34.145	-8.395	1.00	35.82	Α
	ATOM	1764	CB	PRO A 30		33.571	-7.009	1.00	35.09	A
	ATOM	1765	CG	PRO A 3		32.401	-6.933		34.93	
	ATOM	1766	C	PRO A 3	_	33.506	-9.485	1.00	37.48	Α
	ATOM	1767	ō	PRO A 30		32.504	-10.083		37.30	
45	ATOM	1768	N	ALA A 3			-9.744	1.00	39.16	Α
77	ATOM	1769	CA	ALA A 3	i i		-10.775		39.50	
	ATOM	1770	CB	ALA A 3	·		-10.640		39.58	
	ATOM	1771	C	ALA A 3		_	-10.832	1.00	41.05	Α
	ATOM	1772	o	ALA A 3			-11.920	1.00	42.39	Α
50	ATOM	1773	N	ALA A 3				1.00	40.38	Α
50	MOTA	1774		ALA A 3	_			1.00	39.93	A
	MOTA	1775	CB	ALA A 3					41.64	
		1776	G	ALA A 3			-10.002		38.27	
	MOTA MOTA	1777	0	ALA A 3			-10.453		39.29	
55	ATOM	. 1778	N	PHE A 3					35.83	
ככ	ATOM	1779	CA	PHE A 3			-10.085		33.62	
	ATOM		CB	PHE A 3	_		-10.278	1.00	32.70	Α
	ATOM	1781		PHE A 3					31.41	
	ATOM	1782		PHE A 3			-10.574		30.30	
	TION	± / U Z								

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	MOTA	1783	CD2	PHE	A :	305	96.556	29.225	-8.562	1.00 30.99 A
	MOTA	1784	CE1	PHE	A	305	95.230	27.350	-10.136	1.00 29.76 A
	ATOM	1785	CE2	PHE	A	305	95.352	28.663	-8.105	1.00 30.08 A
	ATOM	1786	CZ	PHE	Α	305	94.689	27.725	-8.897	1.00 30.22 A
5	MOTA	1787	. C	PHE	A	305	99.735	27.580	-11.241	1.00 32.03 A
	ATOM	1788	0	PHE	Α	305	99.767	27.962	-12.405	1.00 32.54 A
	ATOM	1789	N	PHE	Α	306	99.781	26.290	-10.914	1.00 31.58 A
	ATOM	1790	CA	PHE			99.886	25.235	-11.932	1.00 30.32 A
	ATOM	1791	СВ	PHE			99.518		-11.338	1.00 29.86 A
10	ATOM .	1792	CG	PHE			100.087	23.639	-9.971	1.00 30.29 A
	ATOM	1793		PHE			101.447	23.783	-9.733	1.00 30.37 A
	ATOM	1794		PHE			99.259	23.275	-8.919	1.00 30.23 A
	ATOM	1795		PHE			101.975	23.570	-8.465	1.00 30.98 A
	ATOM	1796		PHE			99.773	23.061	-7.648	1.00 30.91 A
15	ATOM	1797	CZ	PHE			101.136	23.210	-7.418	1.00 31.14 A
13		1798	C	PHE			98.949		-13.096	1.00 29.48 A
	ATOM			PHE			97.738		-12.920	1.00 30.39 A
•	ATOM	1799	N O	PRO			99.501		-14.309	1.00 28.76 A
	MOTA	1800					100.934		-14.635	1.00 27.67 A
20	ATOM	1801	CD	PRO					-15.520	1.00 27.24 A
20	MOTA	1802	CA ·	PRO			98.731			1.00 27.24 A 1.00 25.23 A
	ATOM	1803	CB	PRO			99.757		-16.635	· ·
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	MOTA	1805	C	PRO			97.457		-15.787	
	MOTA	1806	0	PRO			96.419		-16.098	1.00 24.65 A
25	MOTA	1807	И	LYS					-15.682	1.00 25.13 A
	MOTA	1808	CA	LYS			96.330		-15.952	1.00 24.53 A
	MOTA	1809	CB	LYS			96.689		-16.136	1.00 24.86 A
	MOTA	1810	CG	LYS			97.361		-17.490	1.00 25.50 A
	MOTA	1811	CD	LYS			97.987		-17.616	1.00 27.33 A
30	MOTA	1812	CE	LYS	Α	308	98.678		-18.961	1.00 29.39 A
	MOTA	1813	NZ	LYS			99.232		-19.146	1.00 32.38 A
	MOTA	1814	C	LYS	Α	308	95.282		-14.890	1.00 24.82 A
	MOTA	1815	0	LYS	Α	308	94.085		-15.193	1.00 24.89 A
	MOTA	1816	N	ALA	Α	309	95.716		-13.647	1.00 24.73 A
35	MOTA	1817	CA	ALA	Α	309	94.758	23.716	-12.573	1.00 25.03 A
	MOTA	1818	CB	ALA	Α	309	95.445	23.662	-11.208	1.00 24.10 A
	MOTA	1819	C	ALA	Α	309	94.140	25.094	-12.816	1.00 25.34 A
	MOTA	1820	0	ALA	Α	309	92.934	25.273	-12.679	1.00 26.34 A
	MOTA	1821	\mathbf{N}	ARG	A	310	94.958	26.067	-13.198	1.00 26.07 A
40	MOTA	1822	CA	ARG	A	310	94.419	27.396	-13.453	1.00 28.32 A
	MOTA	1823	CB	ARG	Α	310	95.513	28.359	-13.908	1.00 29.31 A
	ATOM	1824	CG	ARG	Α	310	94.940	29.708	-14.288	1.00 31.58 A
	MOTA	1825	CD	ARG	Α	310	95.917	30.588	-15.030	1.00 31.47 A
	MOTA	1826	NE	ARG	A	310	95.275	31.825	-15.473	1.00 34.52 A
45	ATOM	1827	CZ	ARG	Α	310	95.771	33.050	-15.276	1.00 35.51 A
	MOTA	1828	NH1	ARG	Α	310	96.929	33.205	-14.633	1.00 33.99 A
	ATOM	1829	NH2	ARG	Α	310	95.106	34.124	-15.720	1.00 32.10 A
	ATOM	1830	С	ARG			93.331	27.348	-14.521	1.00 29.03 A
	ATOM	1831	0	ARG	Α	310	92.308	28.034	-14.418	1.00 29.32 A
50	ATOM	1832	N	ASP			93.548	26.536	-15.551	1.00 29.06 A
- •	ATOM	1833	CA			311			-16.620	1.00 29.87 A
	MOTA	1834	CB	ASP			93.156	•	-17.776	1.00 31.71 A
	ATOM	1835	CG	ASP			92.207		-18.953	1.00 34.71 A
	ATOM	1836		ASP			91.288		-18.912	1.00 36.90 A
55	ATOM	1837		ASP			92.378		-19.918	1.00 36.33 A
55	ATOM	1838	C	ASP			91.264		-16.128	1.00 29.70 A
	ATOM	1839	0	ASP			90.169		-16.513	1.00 29.95 A
		1840	N	LEU			91.383		-15.282	1.00 26.64 A
	ATOM	1841	CA	LEU			90.215		-14.715	1.00 24.92 A
	ATOM	TOAT	CA		~		20.22			•

	ATOM	1842	CB	LEU A	312	•	90.645	22.911	-13.869	1.00	23.93	Α
	ATOM	1843	CG	LEU A	312		89.504	22.112	-13.227	1.00	24.48	Α
	ATOM	1844	CD1	LEU A	312		88.569	21.610	-14.296	1.00	25.07	Α
	ATOM	1845	CD2	LEÙ A	312		90.061	20.945	-12.460	1.00	25.13	A
5	ATOM	1846	C	LEU A	312		89.412	25.095	-13.841	1.00	23.85	Α
•	ATOM	1847	ō	LEU A			88.182		-13.896		21.21	
	ATOM	1848	N	VAL A			90.121		-13.042	1.00	23.12	A
	MOTA	1849	CA	VAL A			89.484		-12.171		23.55	
	ATOM	1850	СВ	VAL A			90.536		-11.297		22.33	
10	ATOM	1851		VAL A			89.898		-10.559		19.05	
10	ATOM	1852		VAL A			91.144		-10.305		19.89	
	ATOM	1853	C	VAL A			88.701		-12.975		25.59	
	ATOM	1854	0	VAL A			87.590		-12.605		26.57	
	ATOM	1855	И	GLU A			89.278		-14.076		26.08	
15		1856	CA	GLU A			88.598		-14.895		26.79	
13	ATOM		CB	GLU A			89.543		-15.948		27.50	
	ATOM	1857	CG	GLU A			90.739		-15.381		32.29	
	ATOM	1858							-16.463		35.85	
	ATOM	1859		GLU A							38.06	
20	ATOM	1860		GLU A			91.967		-17.375		38.48	
20	ATOM	1861		GLU A		•	92.157		-16.399		26.22	
•	ATOM	1862	C	GLU A			87.370		-15.577			
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	ATOM	1864	N	LYS A			87.300		-15.662		24.74	
	ATOM	1865	CA	LYS A			86.151		-16.294		23.60	
25	ATOM	1866	CB	LYS A			86.578		-17.073		23.69	
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	ATOM	1868	·CD	LYS A			87.825		-18.968		25.68	
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30	ATOM	1871	C	LYS A			85.119		-15.230		23.42	
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25	ATOM	1875	CB	LEU A					-12.078		21.14	
35	ATOM	1876	CG	LEU A			85.409		-11.009		19.21	
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40	ATOM	1880	0	LEU A			82.811 84.865		-11.955		20.59	
40	ATOM	1881	N	LEU A		•			-12.175		21.64	
	ATOM	1882	CA	LEU A			84.446		-11.646 -10.900		21.42	
	MOTA	1883	CB	LEU A			85.606				21.80	
	MOTA	1884	CG				86.130 87.299	29.892	-9.711		23.09	
4.0	ATOM	1885		LEU A				30.599	-9.047			_
45	ATOM	1886		LEU A			85.031		-8.724		20.34	
	ATOM	1887	C	LEU A			83.940		-12.810			
	ATOM	1888	0	LEU A			84.568		-13.242		23.29	
	MOTA	1889	N.	VAL A			82.786		-13.324		24.06	
	ATOM	1890	CA	VAL A			82.135		-14.436		23.46	
50	MOTA	1891	CB	VAL A			81.829		-15.547		24.32	
	MOTA	1892		VAL A			81.061		-16.670		22.57	
	MOTA	1893		VAL A			83.136		-16.049		20.68	
	MOTA	1894	С	VAL F		•	80.838		-13.918		24.59	
	MOTA	1895	Ο.	VAL			80.050		-13.250		24.86	
55	MOTA	1896	N	LEU A			80.603		-14.215		24.95	
	MOTA	1897	CA	LEU A			79.383		-13.731		25.79	
	ATOM	1898	CB	LEU F			79.379		-14.154		25.38	
	MOTA	1899	CG	LEU F			80.466		-13.417		27.04	
	ATOM	1900	CD1	LEU A	319	٠	80.452	37.421	-13.869	1.00	25.54	A

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	ATOM	1901	CD2	PEA	Α	319	80.241	35.872 -11.907	1.00 23.27 A
	ATOM	1902	С	LEU	Α	319	78.077	32.989,-14.141	1.00 26.05 A
	ATOM	1903	0	LEU	Α	319	77.171	32.819 -13.319	1.00 27.69 A
	ATOM	1904	N			320	77.982	32.580 -15.400	1.00 25.08 A
5	ATOM	1905	CA			320			
,							76.804	31.881 -15.892	1.00 24.00 A
	ATOM	1906	CB			320	76.788	31.907 -17.420	1.00 24.02 A
	ATOM	1907	CG			320	75.597	31.175 -17.996	1.00 27.27 A
	ATOM	1908		ASP			75.009	30.337 -17.271	1.00 29.66 A
	ATOM	1909	OD2	ASP	Α	320	75.253	31.417 -19.175	1.00 30.03 A
10	ATOM	1910	C	ASP	Α	320	76.846	30.427 -15.396	1.00 24.04 A
	ATOM	1911	0	ASP	Α	320	77.661	29.623 -15.846	1.00 25.11 A
	ATOM	1912	N	ALA			75.940	30.094 -14.489	1.00 23.73 A
	ATOM	1913	CA	ALA			75.867	28.770 -13.887	1.00 23.75 A
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15	ATOM	1915	C			321	75.765	27.599 -14.853	1.00 24.90 A
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	ATOM	1917	N	THR	Α	322	75.176	27.834 -16.019	1.00 25.50 A
	ATOM	1918	CA	THR	Α	322	75.008	26.772 -17.011	1.00 24.60 A
	ATOM	1919	CB	THR	Α	322	73.816	27.064 -17.909	1.00 23.09 A
20	ATOM	1920	OG1	THR	Α	322	74.079	28.263 -18.646	1.00 23.74 A
	ATOM	1921		THR			72.568	27.260 -17.080	1.00 20.71 A
	ATOM	1922	C	THR			76.238	26.596 -17.893	1.00 25.71 A
	ATOM	1923	ō	THR			76.230	25.807 -18.832	1.00 25.24 A
	ATOM	1924							
25			N	LYS			77.300	27.331 -17.592	1.00 25.05 A
25	MOTA	1925	CA	LYS			78.526	27.239 -18.366	1.00 26.46 A
	MOTA	1926	CB	LYS			78.972	28.627 -18.823	1.00 28.68 A
	ATOM	1927	CG	LYS	A	323	78.050	29.304 -19.814	1.00 31.27 A
	ATOM	1928	CD	$rac{1}{1}$	Α	323	78.470	29.004 -21.240	1.00 34.38 A
	ATOM	1929	CE	LYS	Α	323	77.850	29.986 -22.243	1.00 35.12 A
30	MOTA	1930	NZ	LYS	Α	323	76.363	29.936 -22.251	1.00 36.71 A
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	ATOM	1932	0	LYS			80.795	26.615 -18.010	1.00 28.51 A
	ATOM	1933	N	ARG			79.372	26.114 -16.360	
	ATOM	1934	CA	ARG					1.00 24.50 A
35	MOTA	1935	CB				80.429	25.524 -15.543	1.00 23.37 A
55	-			ARG			80.087	25.633 -14.049	1.00 23.41 A
	ATOM	1936	CG	ARG			80.233	27.034 -13.520	1.00 21.60 A
	ATOM	1937	CD	ARG			79.594	27.220 -12.173	1.00 21.55 A
	ATOM	1938	NE	ARG	Α	324	79.245	28.624 -11.986	1.00 19.69 A
	ATOM	1939	CZ	ARG	А	324	78.273	29.054 -11.191	1.00 19.84 A
40	ATOM	1940	NH1	ARG	A	324	77.555	28.183 -10.496	1.00 16.83 A
	ATOM	1941	NH2	ARG	Α	324	77.990	30.358 -11.129	1.00 21.41 A
	ATOM	1942	C	ARG	Α	324	80.717	24.085 -15.897	.1.00 22.63 A
	MOTA	1943	0	ARG	Α	324	79.798	23.280 -16.058	1.00 24.44 A
	ATOM	1944	N	LEU			82.000	23.767 -16.023	1.00 20.68 A
45	ATOM	1945	CA	LEU					1.00 20.00 A
	ATOM	1946	CB	LEU			82.414	22.411 -16.352	
	ATOM	1947					83.952	22.330 -16.386	1.00 20.82 A
			CG	LEU			84.596	21.147 -17.131	1.00 23.08 A
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50	ATOM	1950	C ·	LEU	Α	325	81.840	21.454 -15.290	1.00 20.43 A
•	ATOM	1951	0	LEU.	Α	325	82.062	21.633 -14.097	1.00 18.45 A
	ATOM	1952	N	GLY	A	326	81.076	20.456 -15.725	1.00 21.33 A
	ATOM	1953	CA	GLY			80.501	19.513 -14.778	1.00 20.60 A
	ATOM	1954	C	GLY			78.984	19.523 -14.701	1.00 22.39 A
55	ATOM	1955	0	GLY			78.383	18.493 -14.378	1.00 22.59 A
	ATOM	1956	N	CYS			78.358	20.664 -15.009	1.00 22.33 A
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		エフコノ	LA	C10	M	241	76.896	20.771 -14.963	1.00 25.18 A
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	ATOM ATOM	1958 1959	CB SG	CYS			76.453 76.742	22.246 -14.889 23.237 -16.364	1.00 25.79 A 1.00 31.42 A

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	ATOM	2192	CD	PRO			98.083	11.340	-2.567	1.00 27.35 A
	ATOM	2193	CA	PRO			100.276	11.213	-1.539	1.00 28.63 A
	ATOM	2194	СВ	PRO			100.261	12.199	-2.712	1.00 29.02 A
	ATOM	2195	CG	PRO			98.815	12.633	-2.712	1.00 27.44 A

	ATOM	2196	С	PRO	A	356	100.483	11.899	-0.195	1.00	29.18 A
	ATOM	2197	0	PRO	А	356	99.543	12.505	0.331		28.80 A
	MOTA	2198	N	ALA	Α	357	101.689	11.806	0.368		29.69 A
	MOTA	2199	CA	ALA	Α	357	101.942	12.439	1.664		31.97 A
5	MOTA	2200	CB	ALA	Α	357	103.273	11.964	2.253		29.11 A
	MOTA	2201	С	ALA	А	357	101.928	13.964	1.528		33.61 A
	MOTA	2202	0	ALA			102.371	14.507	0.520		33.81 A
	MOTA	2203	N	LEU			101.390	14.645	2.540		36.37 A
	MOTA	2204	CA	LEU			101.295	16.110	2.543		38.03 A
10	MOTA	2205	CB.	LEU			99.995	16.554	3.209		36.49 A
	MOTA	2206	CG	LEU			98.679	16.059	2.641		35.57 A
	MOTA	2207		LEU			97.568	16.398	3.620		35.78 A
	MOTA	2208	CD2	LEU			98.443	16.689	1.278		37.10 A
	MOTA	2209	С	LEU			102.460	16.743	3.310		39.05 A
15	MOTA	2210	0	LEU			102.451	16.592	4.553		39.24 A
	MOTA	2211		LEU			103.348	17.370	2.679		40.12 A
	MOTA	2212	OH2	TIP		1	82.347	32.462	-3.850		16.08 S
	MOTA	2213	OH2		S	4	80.761		-18.244		23.37 S
	MOTA	2214	OH2	TIP		7	79.269	13.051			22.32 5
20	MOTA	2215	OH2	TIP	S	8	86.710	32.919	-1.646		24.05 S
	ATOM	2216	OH2	TIP		9	78.564	-0.823	16.465		28.00 S 18.43 S
	ATOM	2217	OH2	TIP		10	75.323	16.274	8.538		18.43 S 27.08 S
	ATOM	2218	OH2		S	12	78.540	24.328	-2.128		27.06 S
	MOTA	2219	OH2	TIP		13	91.533		-17.231		23.98 S
25	MOTA	2220	OH2	TIP		14	77.419	-0.445	24.044 -3.114		21.78 S
	MOTA	2221	OH2	TIP	S	19	72.498	40.164	-15.393		22.49 S
	ATOM	2222	OH2	TIP	S	20 21	77.303 75.600	-1.063	22.040		24.29 S
	MOTA	2223	OH2 OH2	TIP	S	22	90.133	19.697	12.606		16.61 S
30	ATOM	2224	OH2	TIP	S	24	74.810	7.002	5.700		20.66 S
30	ATOM	2225 2226	OH2	TIP		27	74.814	8.778	-8.074		23.31 S
	ATOM	2227	OH2	TIP	S	28	80.070		-17.170		27.29 S
	MOTA MOTA	2228	OH2	TIP	S	31	74.744	21.007	3.348		29.98 S
	MOTA	2229	OH2	TIP		32	97.930	12.301	2.472		16.75 S
35	ATOM	2230	OH2	TIP	s	35	78.412	7.338	3.002		16.51 S
33	ATOM	2231	OH2	TIP	s	36	80.172	27.171	1.300	1.00	34.66 S
	ATOM	2232	OH2	TIP	s	41	69.773	3.412	17.444	1.00	24.08 S
	ATOM	2233	OH2	TIP	s	43	88.878	7.904	10.616	1.00	20.34 S
	MOTA	2234	OH2	TIP	s	44	87.375	32.487	-13.928	1.00	31.99 S
40	ATOM	2235	OH2		s	45	91.671	10.803	-16.123		35.59 S
	MOTA	2236	OH2	TIP	s	46	87.637	11.564	23.703	1.00	22.67 S
	ATOM	2237	OH2	TIP	s	48	93.353	28.739	3.547	1.00	32.79 S
	MOTA	2238	OH2	TIP	S	50	82.283	34.597	16.032		23.90 S
	ATOM	2239	ОН2	TIP	s	52	81.673	8.965	-8.348		27.83 S
45	MOTA	2240	OH2	TIP	s	55	94.012	3.488	1.399		24.78 S
	MOTA	2241	OH2	TIP	s	58	85.735	11.257	-18.436		27.15 S
	MOTA	2242		TIP		61	79.069	-4.638	12.345		21.04 S
	MOTA	2243	OH2	TIP	s	64	103.981	17.563	-7.228		28.86 S
	MOTA	2244	OH2	TIP	s	66	79.020	43.119	5.431		33.30 S
50	MOTA	2245	OH2	TIP	S	69	88.177	36.956	3.079		30.87 S
	MOTA	2246	OH2	TIP	S	75	78.707	27.486	-3.439		25.25 S
	MOTA	2247	OH2	TIP	S	79	80.347	33.345	6.422		38.57 S
	ATOM	2248	OH2	TIP	S	84	64.594	19.493	24.406		26.01 S
	MOTA	2249	OH2			98	70.215	21.980	19.413		24.75 S
55	MOTA	2250		TIP			103.456	14.637	-2.925		41.84 S
	MOTA	2251	OH2				97.528	14.189	-14.706		43.27 S
	MOTA	2252		TIP			103.602	10.418	-1.388		37.07 S
	MOTA	2253		TIP			83.353	33.273	4.410		34.78 S
	MOTA	2254	OH2	TIP	S	130	74.116	4.597	-3.022	Τ.00	27.69 S

	MOTA	2255	OH2	TIP	s	131	73.104	-1.689	21.760	1.00 32.76 S
	MOTA	2256	OH2	TIP	S	133	101.510	19.036	-1.083	1.00 28.30 S
	ATOM	2257	OH2	TIP	s	134	65.138	6.209	20.472	1.00 27.43 S
	MOTA	2258	OH2	TIP	s	135	94.509	36.623	-12.734	1.00 40.27 S
5	MOTA	2259	OH2	TIP	s	136	76.896	11.412	-17.698	1.00 37.17 S
	ATOM	2260	OH2	TIP	S	137	97.379	7.497	-6.673	1.00 41.53 S
	ATOM	2261	OH2	TIP		138	62.239	17.934	24.368	1.00 34.35 S
	ATOM	2262		TIP		139	69.630		-10.771	1.00 38.17 S
	ATOM	2263		TIP		140	84.554	44.493	-2.658	1.00 24.74 S
10	ATOM	2264		TIP		141	94.631	8.129	-9.752	1.00 35.45 S
10	ATOM	2265		TIP		142	78.415	1.021	3.883	1.00 28.60 S
	ATOM	2266		TIP		143	99.830	12.987		1.00 25.00 S
		2267		TIP		144	71.235	20.688	11.365	1.00 55.75 S
•	ATOM			TIP						1.00 31.32 S
1.5	ATOM	2268				145	87.138	25.623	11.165	
15	ATOM	2269		TIP		146	60.803	15.332	23.294	1.00 32.69 S
	ATOM	2270		TIP		148	73.970		-13.455	1.00 33.99 S
	ATOM	2271		TIP		149	88.146	19.004	17.326	1.00 27.60 S
	MOTA	2272		TIP		150	90.803	9.970	18.127	1.00 35.03 S
	ATOM	2273		TIP		153	86.261	32.393		1.00 41.89 S
20	MOTA	2274		TIP		155	102.147	7.767	-0.215	1.00 38.83 S
	MOTA	2275	OH2	TIP		159	95.238	0.811	-7.614	1.00 47.22 S
	MOTA	2276	× .	TIP		163	92.356	36.543	-5.580	1.00 40.19 S
	MOTA	2277	OH2	TIP	s	172	66.640	4.633	22.314	1.00 29.95 S
	MOTA	2278	OH2	TIP	S	176	99.303	9.124	3.136	1.00 37.07 S
25	MOTA	2279	OH2	TIP	s	184	104.566	20.517	-7.318	1.00 40.83 S
	MOTA	2280	OH2	TIP	s	185	90.295	6.390	-15.433	1.00 34.81 S
	MOTA	2281	OH2	TIP	s	186	82.626	12.831	8.023	1.00 23.99 S
	MOTA	2282	OH2	TIP	s	187	86.159	18.737	24.618	1.00 32.12 S
	MOTA	2283	OH2	TIP	s	188	79.867	7.010	-7.877	1.00 28.52 S
30	MOTA	2284	OH2	TIP	s	189	88.469	4.967	1.404	1.00 45.39 S
	MOTA	2285	OH2	TIP	s	190	95.628	28.435	-17.705	1.00 31.73 S
•	MOTA	2286	OH2	TIP	s	191	76.228	7.822	28.547	1.00 36.76 S
	MOTA	2287	OH2	TIP	s	192	85.930	8.936	23.323	1.00 31.58 S
	ATOM	2288	OH2	TIP	s	193	73.669	24.555	-14.317	1.00 34.12 S
35	ATOM	2289	OH2	TIP	s	194	99.847	12.959	4.319	1.00 43.06 S
	ATOM	2290	OH2	TIP		195	76.225	28.669	-3.386	1.00 38.83 S
	ATOM	2291		TIP		197	76.955	24.214	20.057	1.00 35.16 S
	ATOM	2292		TIP		198	65.723	11.313	28.926	1.00 38.40 S
	ATOM	2293	OH2	TIP		199	88.482	28.463	4.472	1.00 29.21 S
40	ATOM	2294	OH2	TIP	S	200	71.017	17.440	-13.980	1.00 37.15 S
	ATOM	2295		TIP		201	64.967	12.265	13.947	1.00 55.03 S
	ATOM	2296	OH2	TIP		204	99.611		-14.818	1.00 46.97 S
	ATOM	2297	OH2	TIP	s	205		-1.944	20.970	1.00 65.13 S
	ATOM	2298	OH2	TIP		210	89.648	5.683	12.672	1.00 38.65 S
45	ATOM	2299		TIP			80.842	40.555	7.721	1.00 37.38 S
73	ATOM	2300		TIP			77.452	22.142	23.411	1.00 37.30 B
	MOTA	2300		TIP			104.280		-10.347	1.00 35.35 B
	ATOM			TIP				44.787	-5.575	1.00 35.13 S
	ATOM	2302					84.900			1.00 30.10 S
50		2303		TIP			74.759	19.808	9.165	1.00 23.87 S
50	ATOM	2304		TIP			76.375	2.991	-2.919	
	ATOM	2305		TIP			97.252	36.990	-15.430	1.00 39.17 S
	ATOM	2306		TIP			70.180	4.692	8.907	1.00 29.97 S
	ATOM	2307		TIP			96.055	11.349	-8.926	1.00 29.40 S
	ATOM	2308		TIP			70.916	31.535	4.186	1.00 53.99 S
55	ATOM	2309		TIP			83.279	23.905	15.245	1.00 40.79 5
	ATOM	2310		TIP			90.441	34.500	3.752	1.00 37.91 S
	ATOM	2311		TIP			74.369		-11.954	1.00 36.85 S
	MOTA	2312		TIP			82.630	5.971	5.382	1.00 48.63 S
	MOTA	2313	OH2	TIP	S	240	101.866	29.649	1.029	1.00 48.93 S

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1.00 58.25 G 74.980 15.310 28.834 2 O12 GLC G MOTA 2314 74.113 15.072 27.724 1.00 58.49 G C11 GLC G 2 MOTA 2315 1.00 58.11 G 74.885 14.362 26.609 2316 C13 GLC G 2 MOTA O14 GLC G 25.524 1.00 58.57 G 73.990 14.120 2 MOTA 2317 1.00 57.55 G C15 GLC G 75.438 13.023 27.096 2 ATOM 2318 74.357 12.183 1.00 57.24 G 27.507 016 GLC G 2 2319 MOTA 1.00 63.76 G 68.191 4.312 13.268 O12 GLC G 3 MOTA 2320 1.00 63.57 G 67.998 3.273 14.231 C11 GLC G 3 MOTA 2321 C13 GLC G 14.330 1.00 64.06 G 3 69.274 2.429 MOTA 2322 1.00 62.75 G O14 GLC G 69.570 1.858 13.049 3 10 ATOM 2323 1.00 63.85 G 15.364 C15 GLC G 69.094 1.303 3 2324 MOTA 0.444 14.978 1.00 65.65 G 016 GLC G 3 68.010 MOTA 2325 87.921 37.473 -13.378 1.00 46.73 G O12 GLC G ATOM 2326 4 36.757 -14.265 1.00 46.84 G C11 GLC G 88.767 4 ATOM 2327 1.00 46.74 G C13 GLC G 4 90.050 36.439 -13.526 15 2328 ATOM 1.00 46.91 G 37.648 -13.104 2329 90.660 MOTA O14 GLC G 4 90.999 35.678 -14.435 1.00 47.60 G C15 GLC G 4 ATOM 2330 1.00 50.48 G 92.193 35.413 -13.700 016 GLC G 2331 4 ATOM 78.608 8.519 28.683 1.00 42.02 G O12 GLC G 6 MOTA 2332 1.00 44.70 G C11 GLC G 6 79.227 8.721 29.956 20 2333 MOTA 1.00 45.13 G C13 GLC G 80.218 9.877 29.849 ATOM 2334 6 81.208 28.896 1.00 47.43 G 9.537 O14 GLC G MOTA 2335 6 80.904 10.129 31.180 1.00 46.92 G C15 GLC G 2336 6 MOTA 1.00 49.38 G 016 GLC G 8.950 31.564 81.611 6 MOTA 2337 1.00 46.74 G 83.278 5.163 12.485 012 GLC G 8 25 2338 MOTA 3.987 12.559 1.00 50.09 G 82.460 2339 C11 GLC G 8 МОТА 1.00 50.09 G 83.236 2.894 13.286 MOTA 2340 C13 GLC G 8 1.00 50.75 G 12.529 84.408 2.621 O14 GLC G ATOM 2341 8 1.00 52.04 G C15 GLC G 82.412 1.597 13.414 8 2342 ATOM 1.00 53.37 G 12.130 ATOM 016 GLC G 8 82.051 1.062 30 2343 1.00 25.46 G -5.006 4.682 012 GLC G 10 87.146 ATOM 2344 85.823 5.086 -5.356 1.00 27.64 G MOTA 2345 C11 GLC G 10 1.00 30.79 G 5.498 -6.835 C13 GLC G 10 85.782 ATOM 2346 1.00 29.47 G -7.069 86.689 6.600 014 GLC G 10 MOTA 2347 84.354 5.916 -7.219 1.00 30.60 G C15 GLC G 10 35 MOTA 2348 1.00 31.23 G 83.947 7.022 -6.417 2349 016 GLC G 10 MOTA 1.00 17.56 L 19.878 9.473 82.223 CBI DRG L MOTA 2350 1 1.00 20.33 L 82.835 19.573 10.730 OBH DRG L 1 2351 **ATOM** 11.733 1.00 17.87 L 20.512 2352 CBG DRG L 1 82.419 MOTA 12.177 1.00 16.47 L 21.291 83.661 40 2353 CBF DRG L 1 MOTA 84.171 22.133 11.085 1.00 15.68 L 2354 NBK DRG L 1 ATOM 1.00 12.47 L 10.751 CBJ DRG L 7 83.683 23.479 ATOM 2355 1.00 16.76 L 12.600 84.739 20.294 CBE DRG L 1 ATOM 2356 13.715 1.00 18.27 L 19.405 CBA DRG L 1 84.178 2357 ATOM 14.017 1.00 18.03 L 82.790 19.632 2358 OBB DRG L 1 45 **ATOM** 81.853 19.747 12.937 1.00 18.62 L 1 CBC DRG L ATOM 2359 1.00 14.59 L CBD DRG L 80.732 20.611 13.524 1 2360 ATOM 1.00 18.60 L 12.551 2361 NAW DRG L 1 81.398 18.547 MOTA 12.014 1.00 15.55 L 80.185 CAX DRG L 1 18.344 MOTA 2362 11.643 1.00 13.82 L 79.107 19.141 1 50 2363 CAY DRG L MOTA 11.053 1.00 16.37 L 77.988 18.555 CAZ DRG L 1 MOTA 2364 1.00 15.88 L 10.830 CAP DRG L 1 77.930 17.180 **ATOM** 2365 11.196 1.00 15.07 L CAO DRG L 1 78.999 16.366 2366 MOTA 1.00.17.80 L 11.783 16.973 CAN DRG L 1 80.107 MOTA 2367 81.290 12.187 1.00 19.34 L 16.377 1 CAM DRG L 55 ATOM 2368 1.00 19.93 L 1 81.811 15.087 12.083 CAH DRG L MOTA 2369 12.657 1.00 18.53 L 1 82.083 17.407 2370 CAV DRG L ATOM 13.014 1.00 18.70 L CAU DRG L 1 83.404 17.144 2371 MOTA 13.438 1.00 17.82 L

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NAT DRG L

ATOM

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	ATOM	2373	CAS	DRG	L	1	85.523	17.317	13.610	1.00	15.80	L
	ATOM	2374	CAR	DRG	L	1	86.807	17.682	14.000	1.00	14.23	L
	ATOM	2375	CAQ	DRG	L	1	87.803	16.708	14.047	1.00	13.92	L
	ATOM	2376	CAI	DRG	L	1	87.526	15.384	13.714	1.00	16.21	L
5	ATOM	2377	CAJ	DRG	L	1	86.244	15.003	13.324			L
	ATOM	2378	CAK	DRG	L	1	85.264	15.988	13.278		17.76	
	ATOM	2379	CAL	DRG	L	1	83.932	15.867	12.904		18.99	
	ATOM	2380		DRG		1	83.130	14.829	12.439		19.47	
	ATOM	2381		DRG		1	83.403	13.472	12.290		18.70	
10	ATOM	2382		DRG		ī	84.471	12.895	12.480		18.10	
	ATOM	2383		DRG		1	82.277	12.904	11.856		18.49	
	ATOM	2384		DRG		1	81.128	13.799	11.622		20.08	
	ATOM	2385	OAF	DRG	L	1	80.902	13.891	10.214		24.92	-
	ATOM	2386	S	S04	I	1	64.638	8.174	16.414			ī
15	ATOM	2387	01	S04	I	1	65.311	9.465	16.666			ī
	ATOM	2388	02	SQ4		1	63.197	8.413	16.200		89.62	
	MOTA	2389	03	S04		1	64.827	7.262	17.566		88.49	
	ATOM	2390	04	SO4	ī	1	65.197	7.555	15.196		89.77	
	ATOM	2391	S	SO4	I	. 3	84.884	-1.751	12.531			Ī
20	ATOM	2392	01	SO4	I	3	84.762	-0.302	12.775			Ī
	ATOM	2393	02	SO4		3	84.538	-2.490	13.758		81.49	
	ATOM	2394	03	SO4	I	3	86.280	-2.053	12.162			ī
	ATOM	2395	04	SO4	ī.		83.976	-2.163	11.440		81.19	
	ATOM	2396	s	SO4	ī	5	74.420	22.898	12.677			Ī
25	ATOM	2397	01	SO4	I	5	73.256	22.153	12.161			ī
	ATOM	2398	02	SO4	I	5	75.637	22.104	12.412		84.51	
	ATOM	2399	03	SO4	I	5	74.250	23.138	14.126			Ī
	ATOM	2400	04	SO4	I	5	74.527	24.202	11.997			Ī
	ATOM	2401	S	SO4	I	6	68.798	6.993	-3.457			Ī
30	ATOM	2402	01	SO4	I	6	68.338	7.338	-4.823			I
	ATOM	2403	02	SO4	I	6	69.298	8.206	-2.791			I
	ATOM	2404	О3	SO4	I	6	69.888	6.003	-3.540			I
	ATOM	2405	04	SO4	I	6	67.690	6.426	-2.658		73.19	I
	ATOM	2406	02	PO4	P	100	66.501	25.721	2.616		85.98	
35 .	ATOM	2407	03	PO4	P	100	64.376	25.028	1.654		86.96	
	ATOM	2408	04	PO4	P	100	65.755	26.653	0.496			р
	ATOM	2409	01	PO4	₽	100	64.621	27.279	2.570		86.98	P
	ATOM	2410	\mathbf{P}	PO4	P	100	65.315	26.170	1.832	1.00	87.36	P
	ATOM	2411	s	504	х	3	80.775	-0.045	7.874	0.50	22.29	Х
40	ATOM	2412	01	SO4	Х	3	81.160	0.521	9.176	0.50	22.30	Х
	ATOM	2413	02	SO4	х	3	81.320	-1.407	7.778		22.49	
	ATOM	2414	03	SO4	х	3	81.309	0.781	6.777		23.26	
	MOTA	2415	04	S04	х	3	79.305	-0.088	7.772		24.36	
	END							•				